Recent Advances in Integrating

Machine Learning and Combinatorial Optimization

Elias B. Khalil

Andrea Lodi

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35th AAAI Conference

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CANADA EXCELLENCE RESEARCH CHAIR
DATA SCIENCE FOR REAL-TIME DECISION-MAKING
UNIVERSITY OF TORONTO
POLYTECHNIQUE MONTRÉAL
USC University of Southern California

Part 1

Introduction to Combinatorial Optimization

Elias Khalil, Andrea Lodi, Bistra Dilkina, Didier Chételat,
Maxime Gasse, Antoine Prouvost, Giulia Zarpellon, Laurent Charlin

MH7: Recent Advances in Integrating
Machine Learning and Combinatorial Optimization

35th AAAI Conference
on Artificial Intelligence
February 3rd 2021

Humans learn to **design** **algorithms**.

Humans learn to **design** **algorithms**.

Can **algorithms** “learn” to **design** **algorithms**?

Humans learn to **design algorithms**.

Machine Learning

Can **algorithms** “learn” to **design algorithms**?

Humans learn to **design algorithms**.

Machine Learning

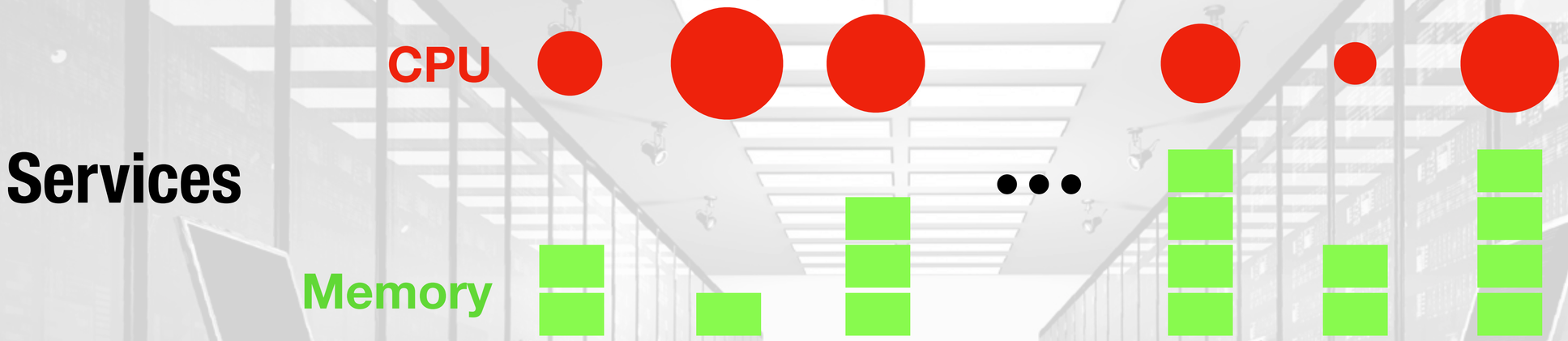
Can **algorithms** “learn” to **design algorithms**?

Combinatorial Optimization

Data Center Resource Management

Photo from: https://www.reit.com/what-reit/reit-sectors/data-center-reits

Data Center Resource Management



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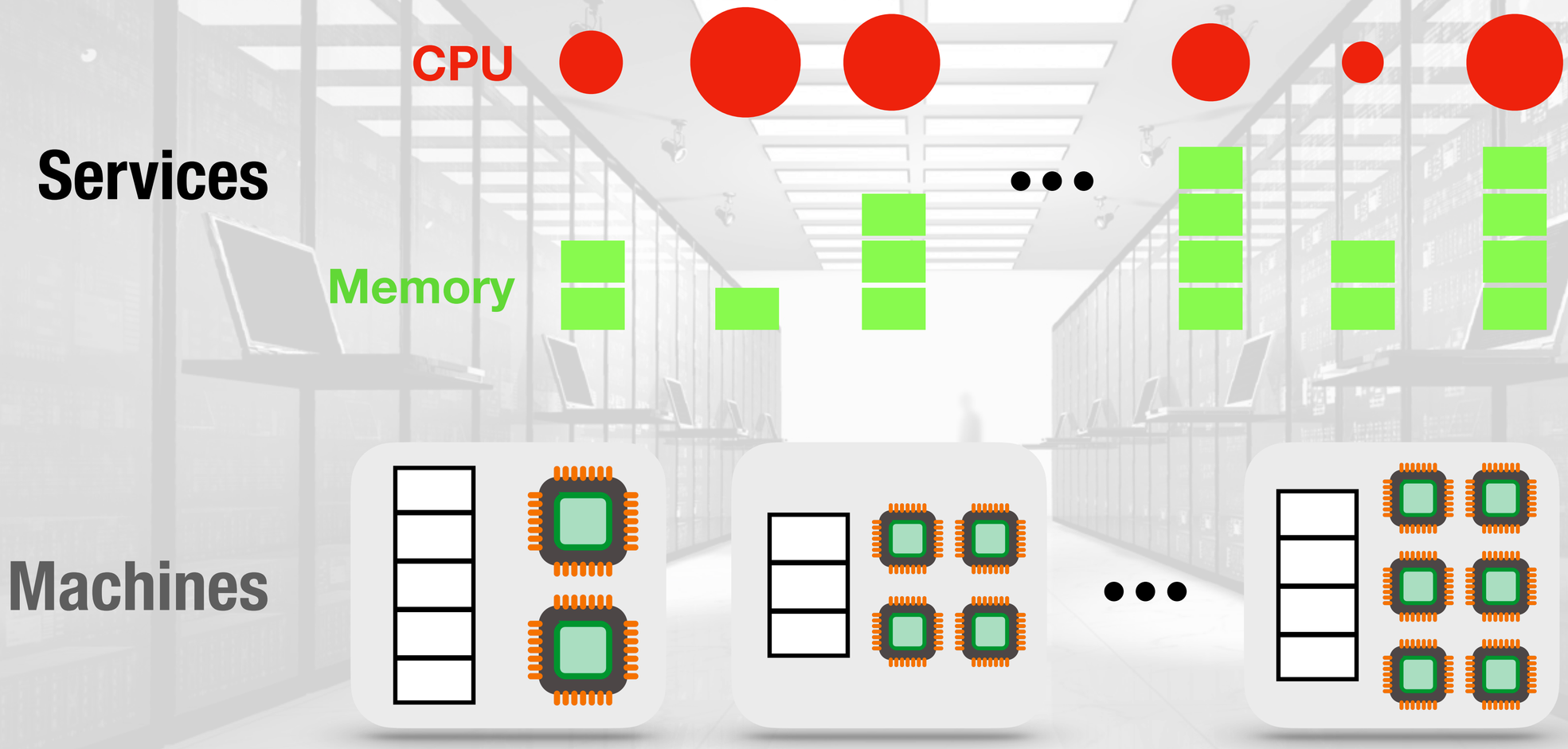

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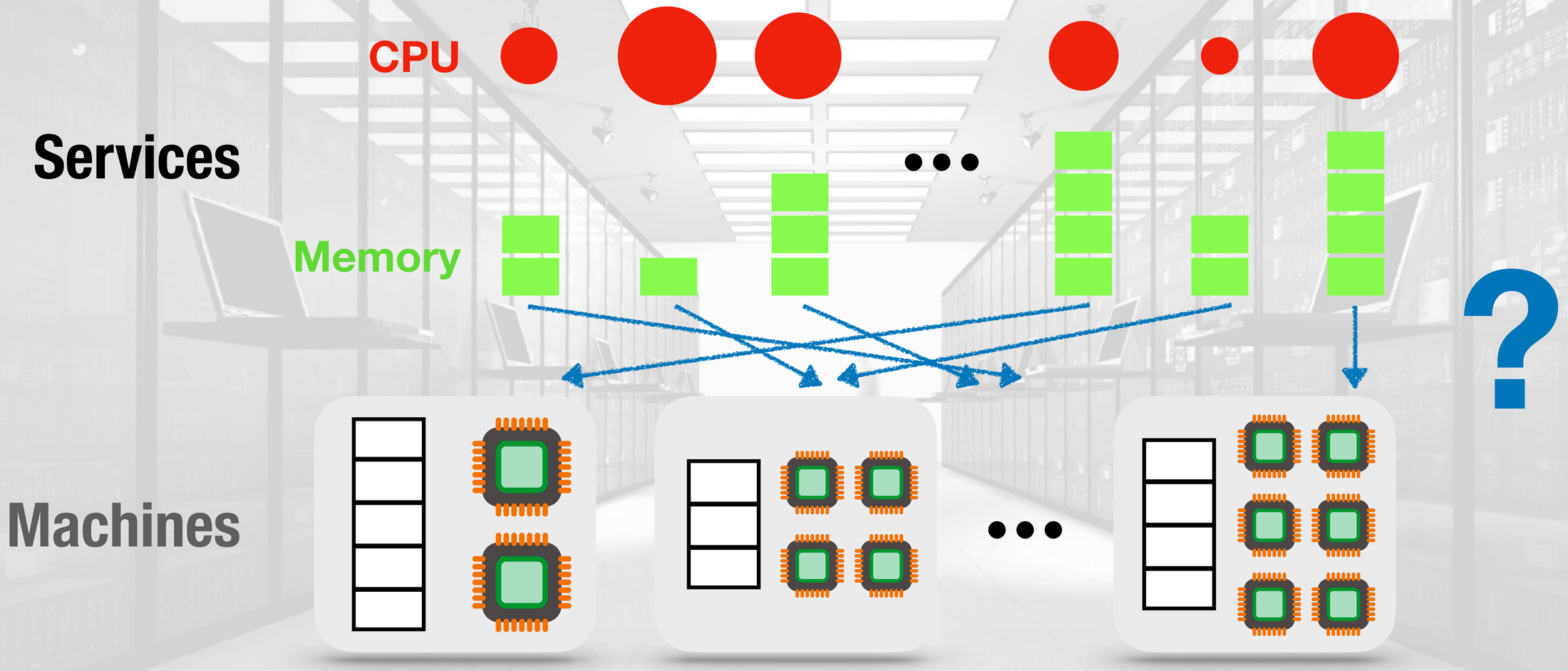

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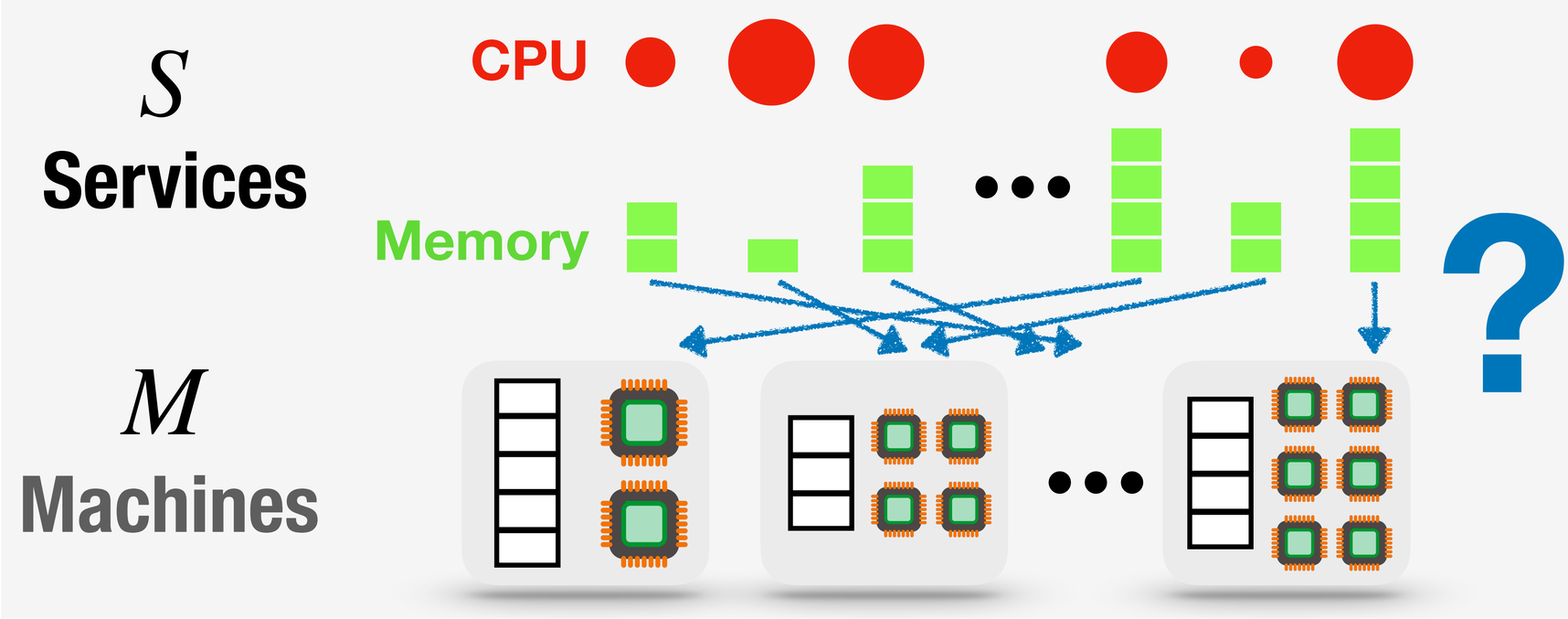
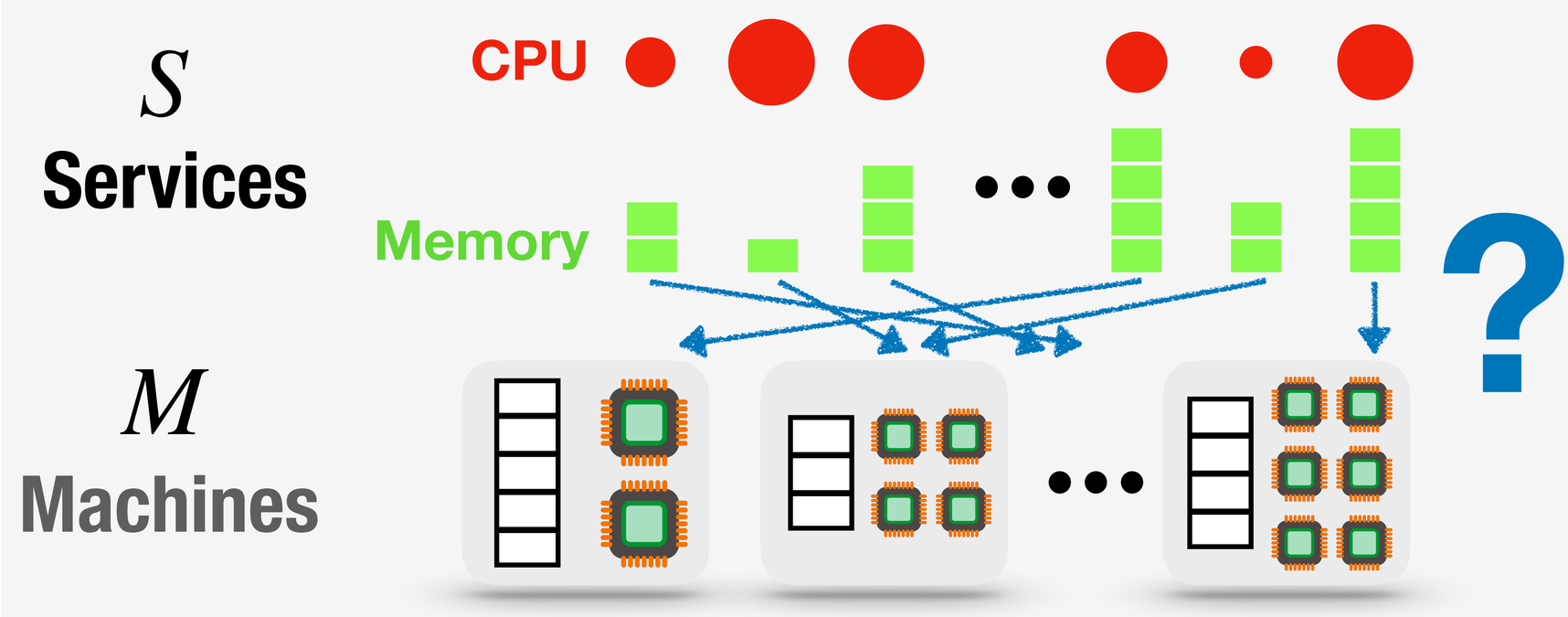

S
Services
CPU
Memory
M
Machines
?

$y_m = 1$ if machine m is used

$x_{s,m} = 1$ if service s runs on m



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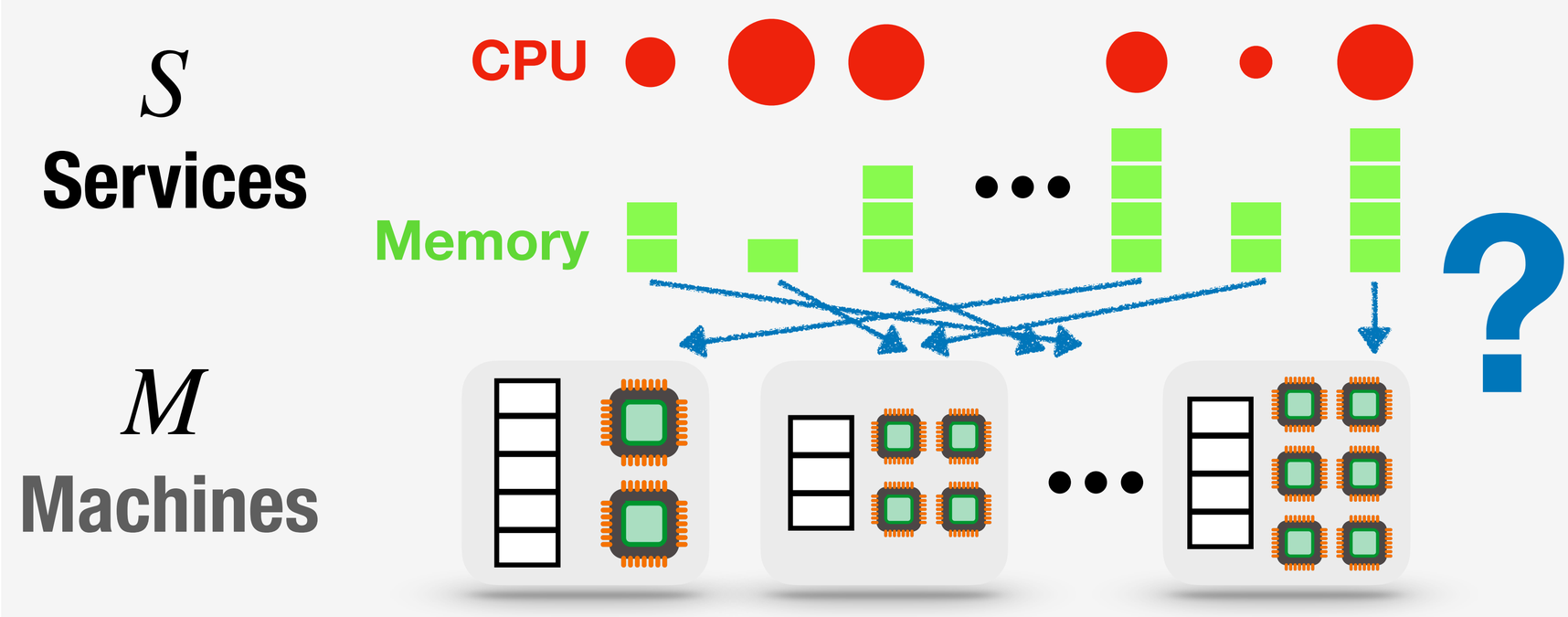

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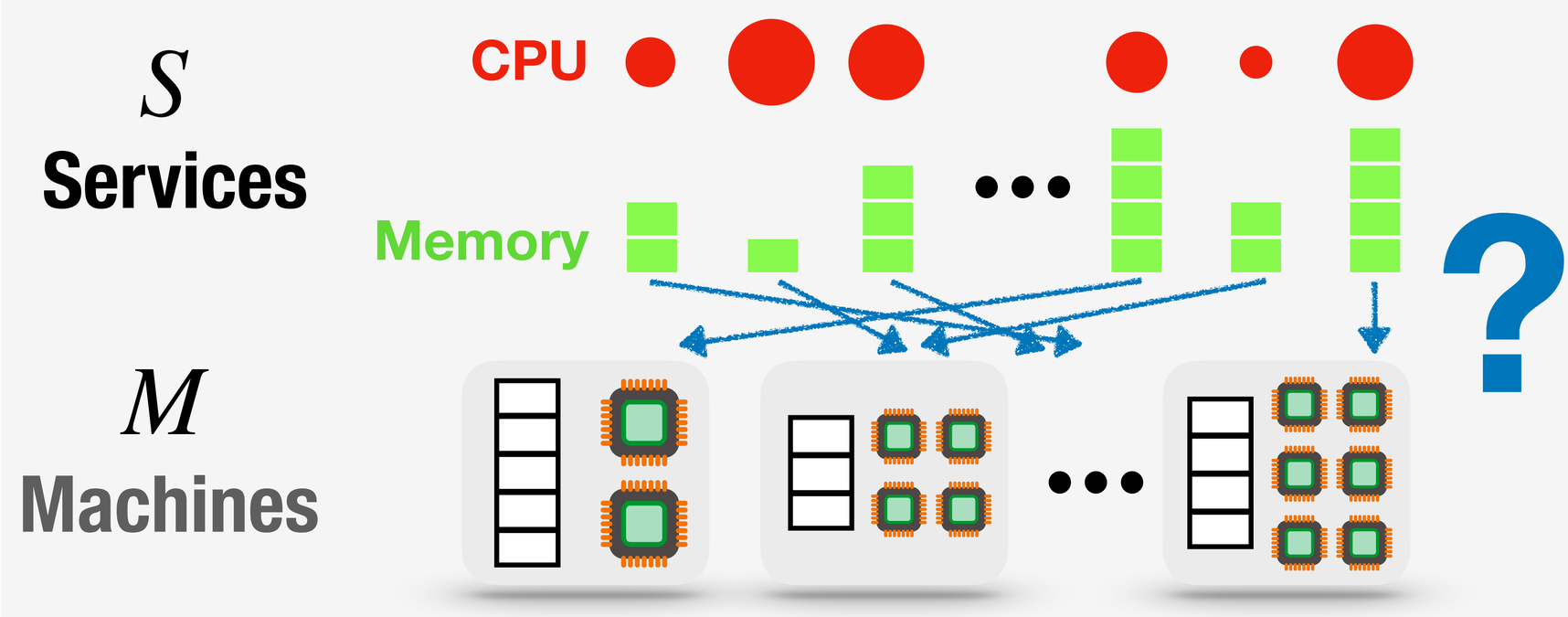

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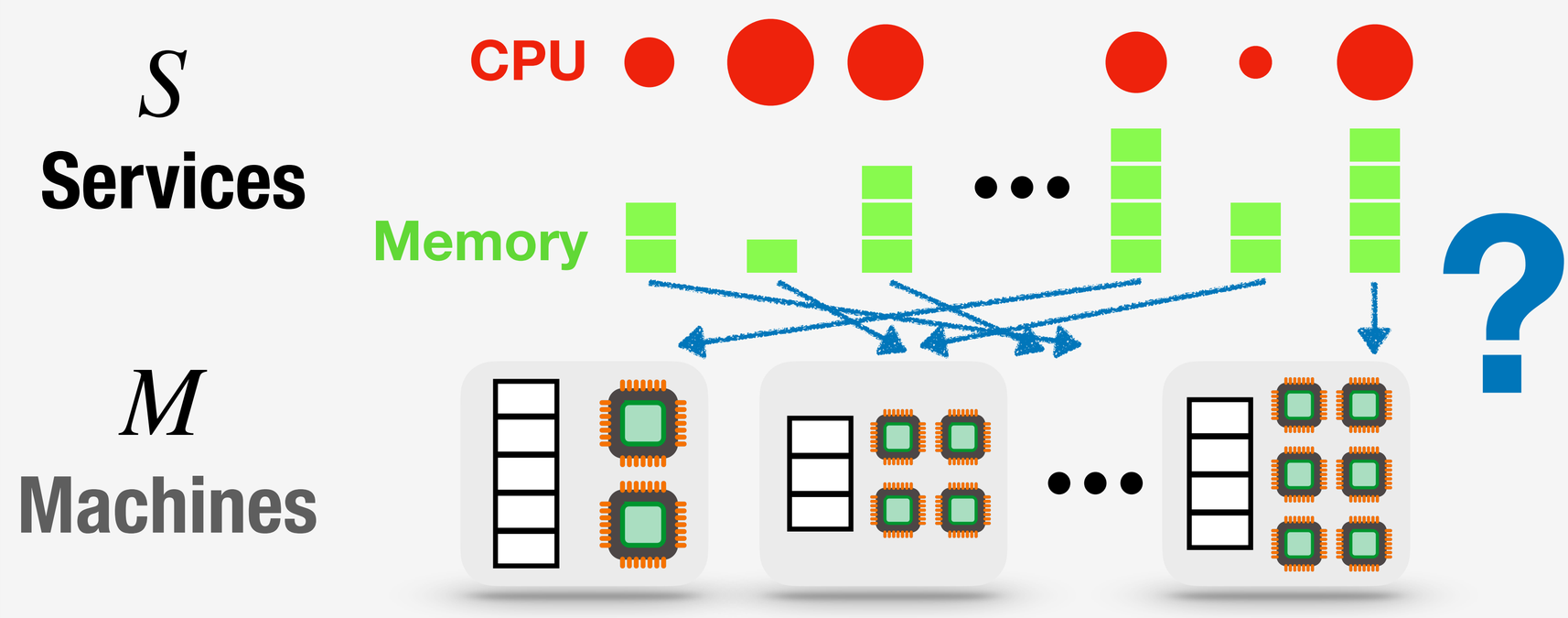

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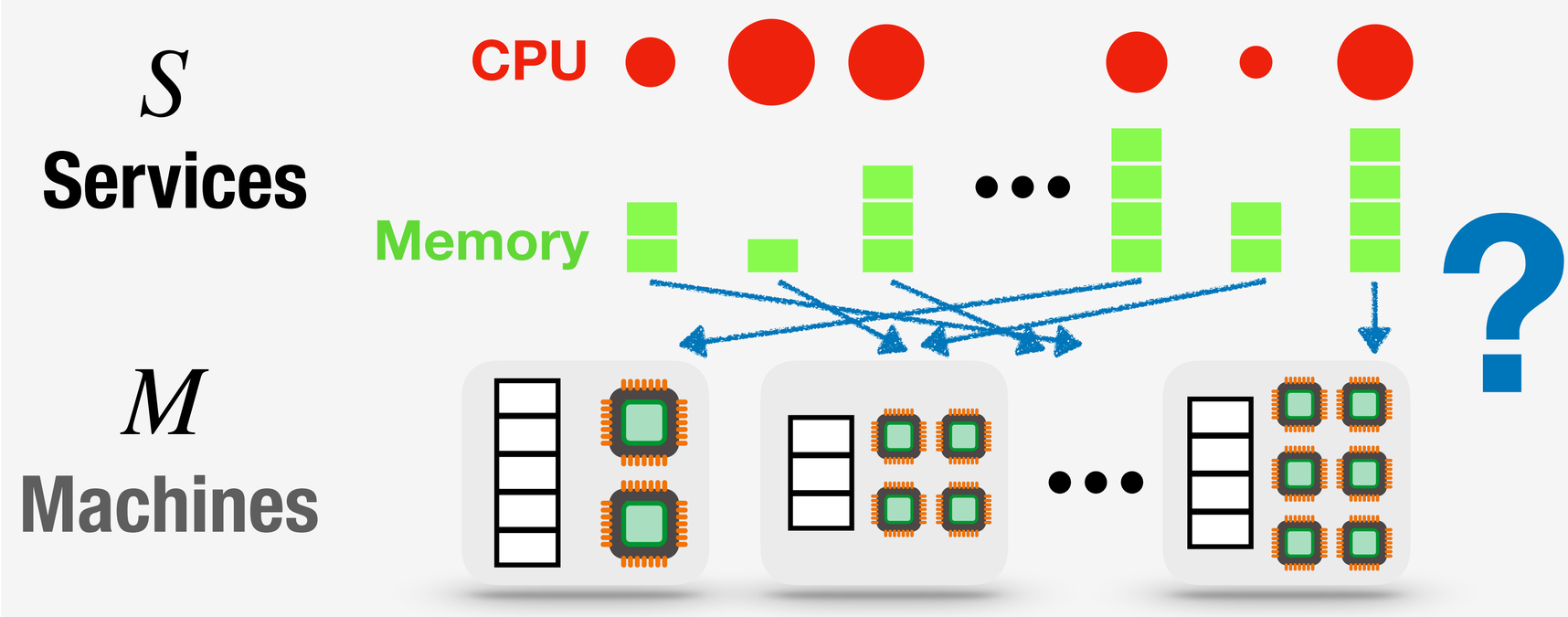
Constraints:

Each service on one machine only

$$\sum_{m=1}^{M} x_{s,m} = 1 \quad \forall s$$



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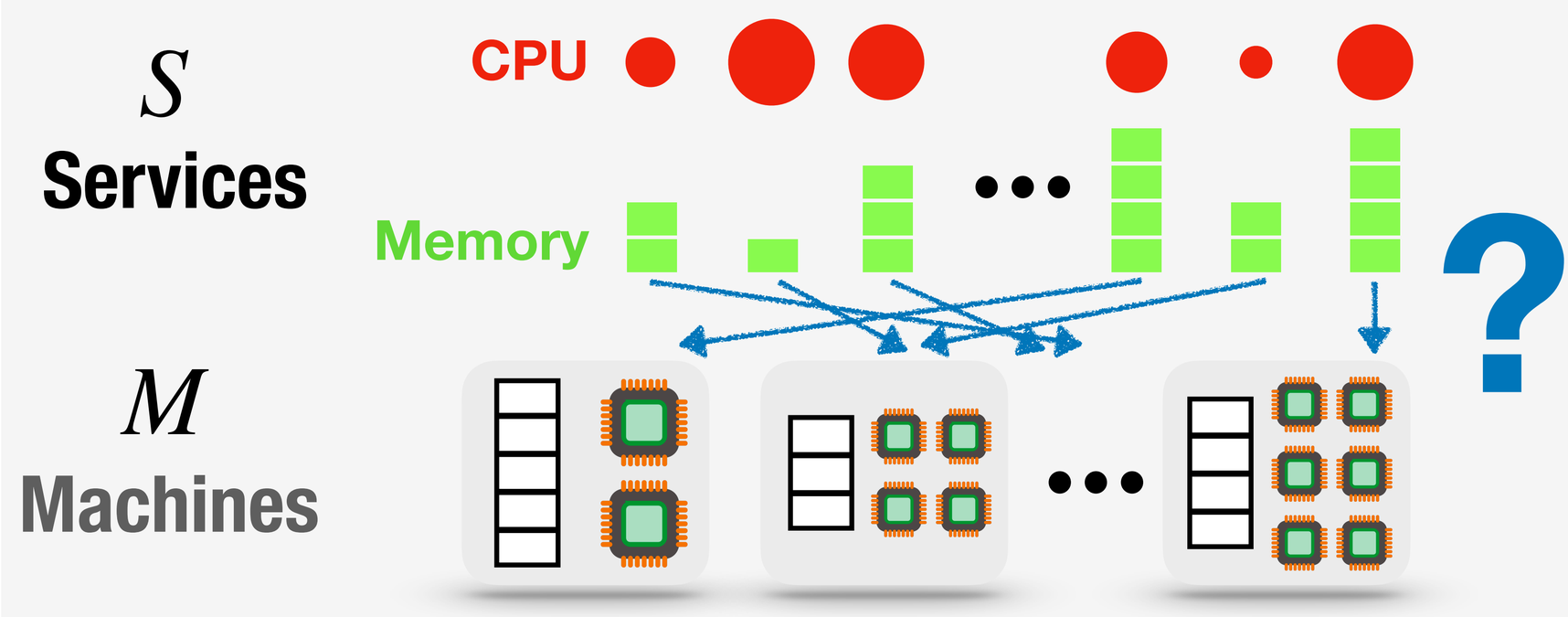

Constraints:

Each service on one machine only

$$\sum_{m=1}^{M} x_{s,m} = 1 \quad \forall s$$

$$y_m \geq x_{s,m} \quad \forall s, m$$

Machine is "ON" if a job is assigned to it

$y_m = 1$ if machine m is used

$x_{s,m} = 1$ if service s runs on m

$x \in \{0,1\}^{S \times M}, y \in \{0,1\}^M$

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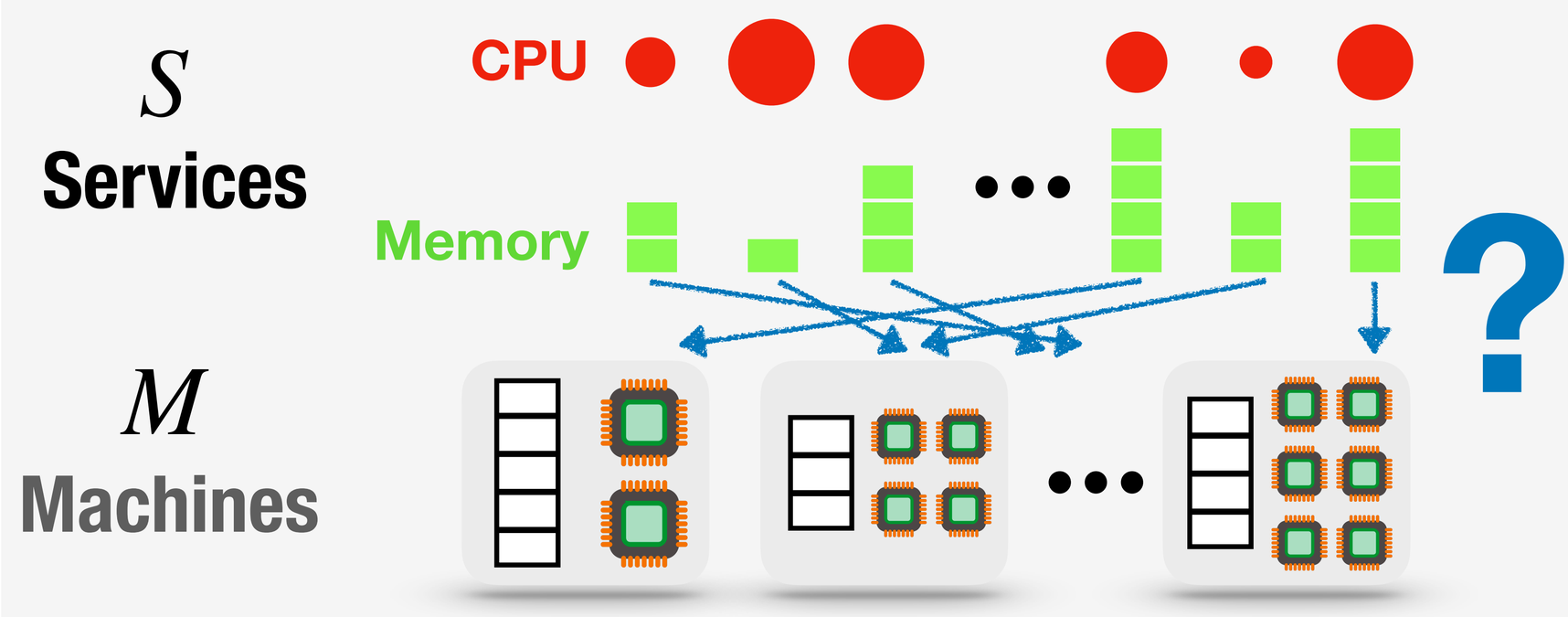

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Each service on one machine only

$$\sum_{m=1}^{M} x_{s,m} = 1 \quad \forall s$$

Memory capacity

$$\sum_{s=1}^{S} \textbf{mem}(s) \cdot x_{s,m} \leq \textbf{cap-mem}(m) \quad \forall m$$

$$y_m \geq x_{s,m} \quad \forall s, m$$

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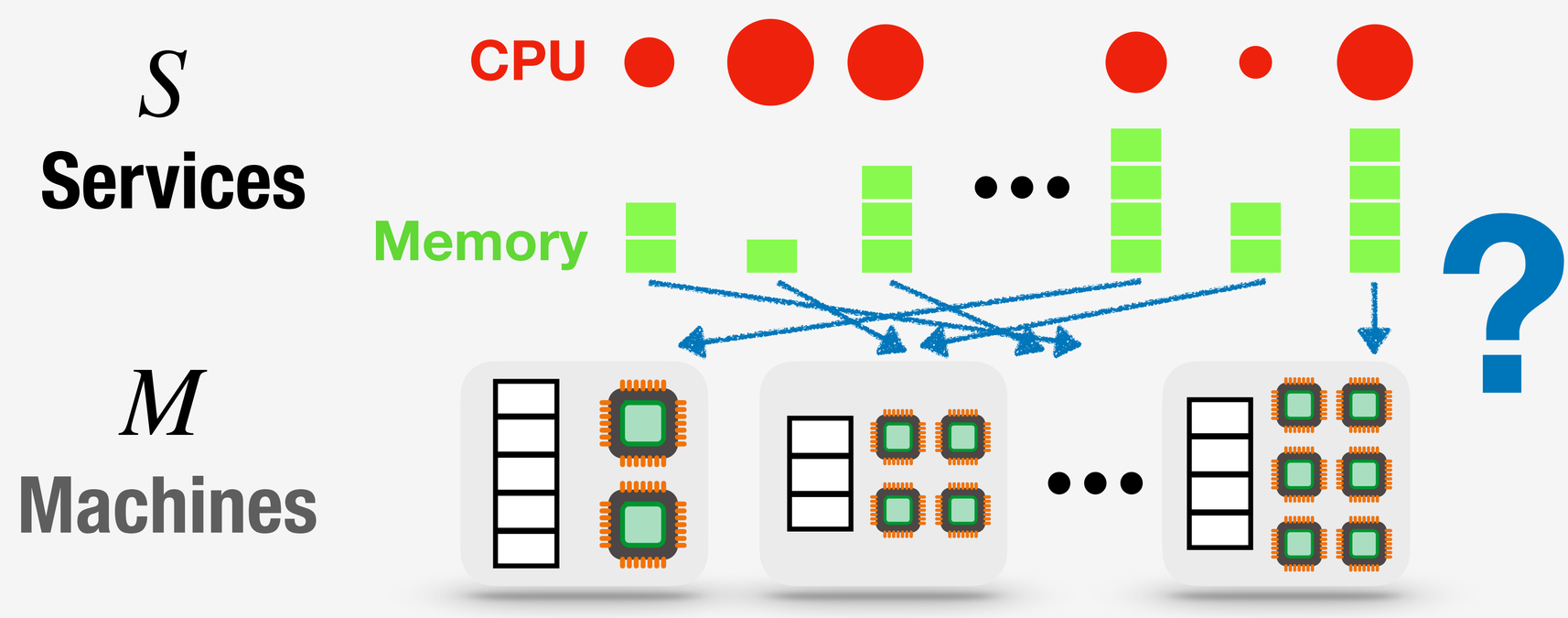

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Machine is "ON" if a job is assigned to it

Memory capacity

$$\sum_{s=1}^{S} \textbf{mem}(s) \cdot x_{s,m} \leq \textbf{cap-mem}(m) \quad \forall m$$

$$\sum_{s=1}^{S} \textbf{cpu}(s) \cdot x_{s,m} \leq \textbf{cap-cpu}(m) \quad \forall m$$

Processor capacity

Safety-Critical Machine Learning

See AAAI-21 Tutorial “AH3: From Explainability to Model Quality and Back Again”

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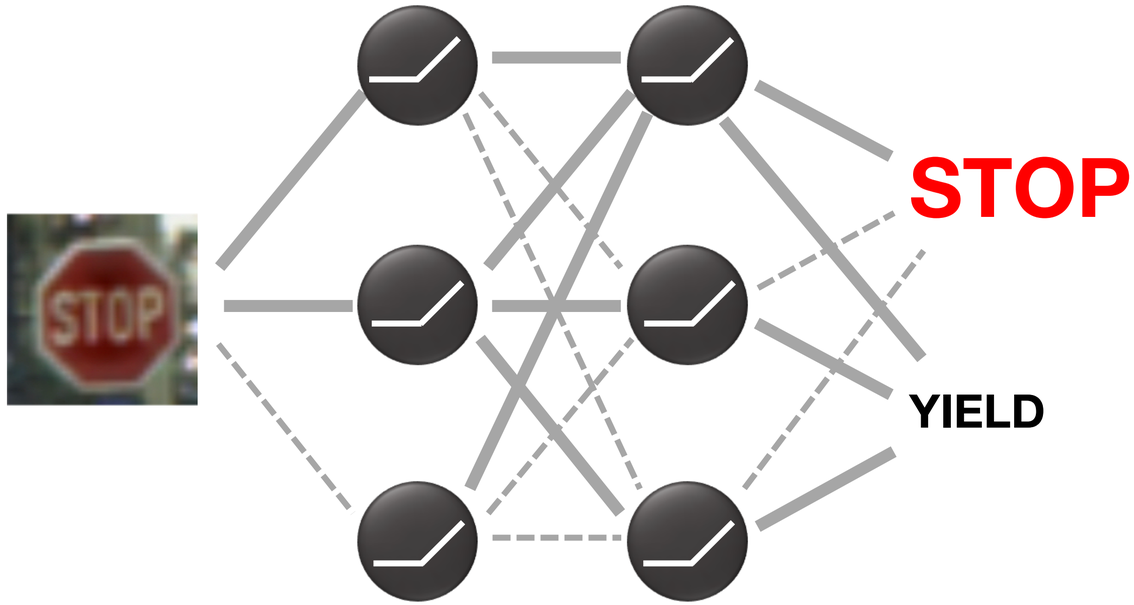

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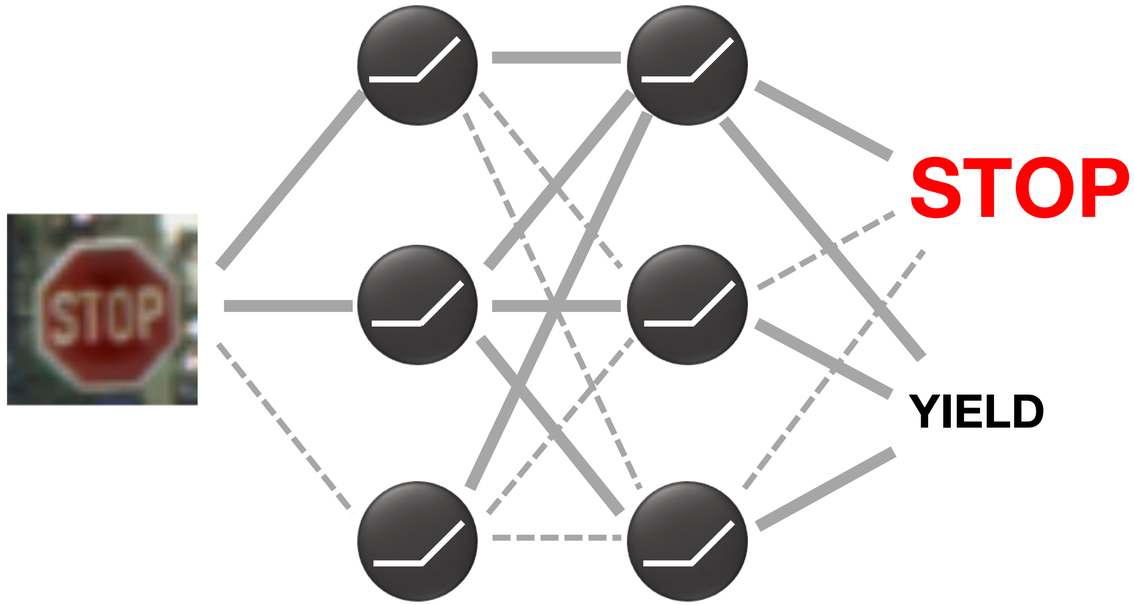

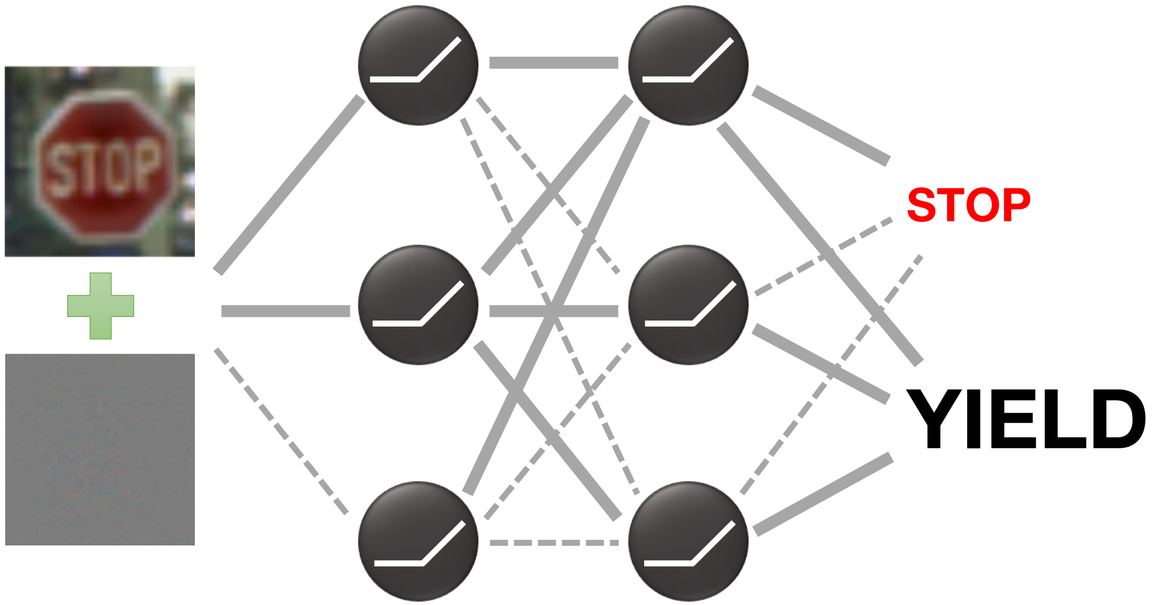

Safety-Critical Machine Learning

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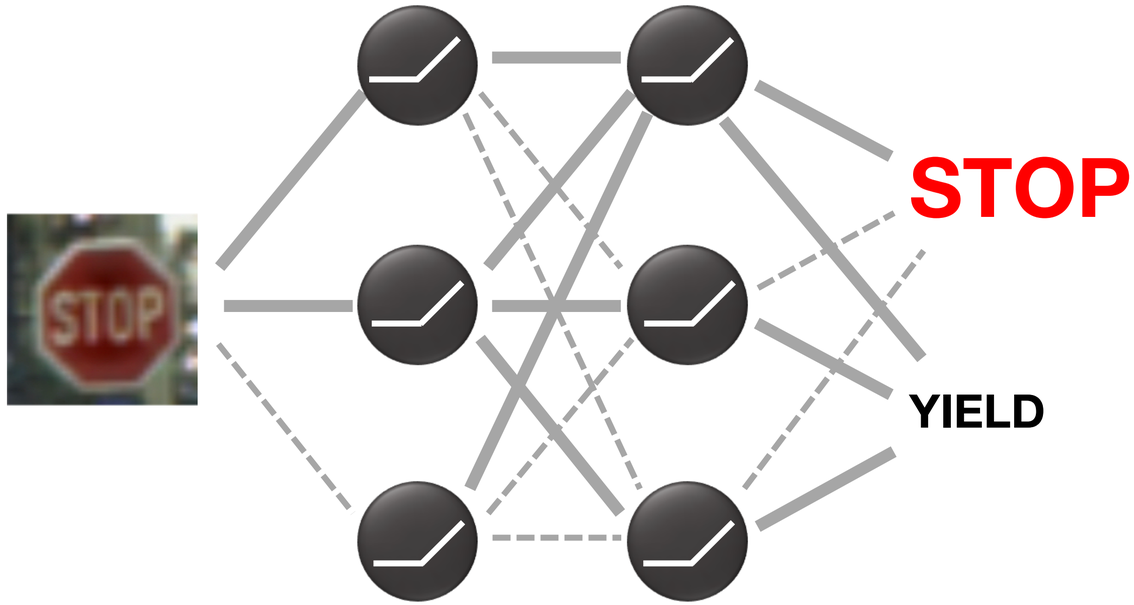
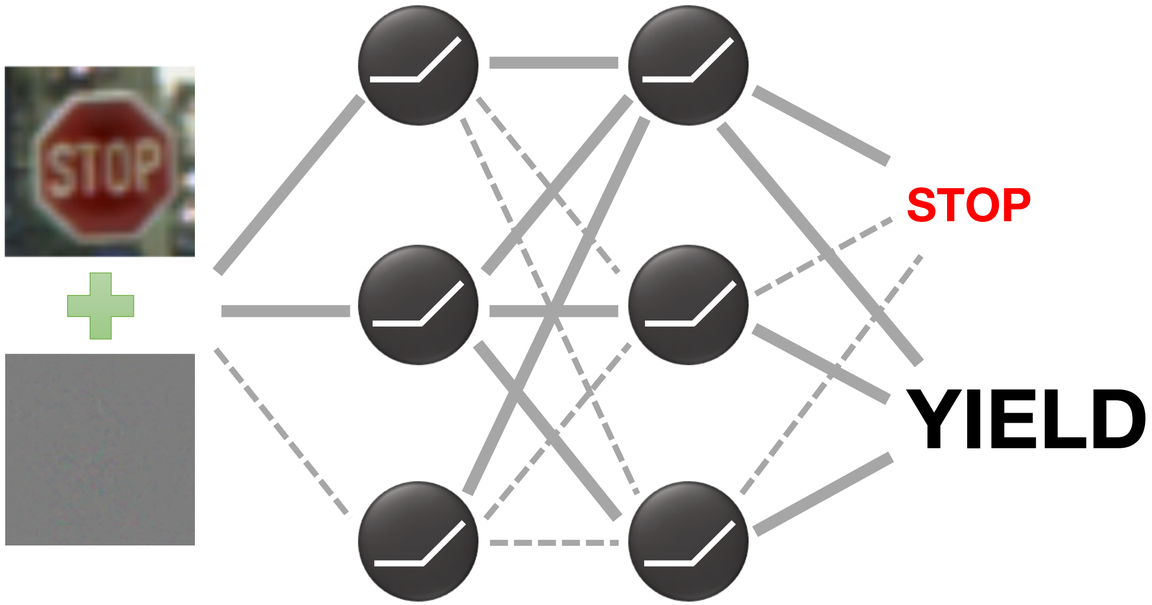
Goal: **Guarantee** that trained model has **desirable behavior**





Safety-Critical Machine Learning

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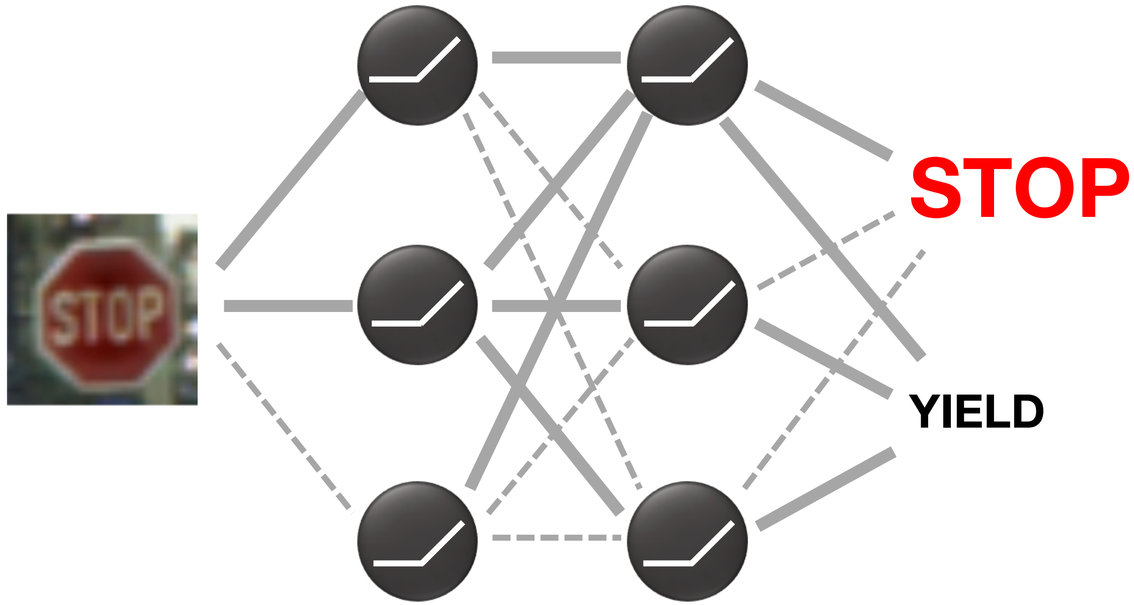
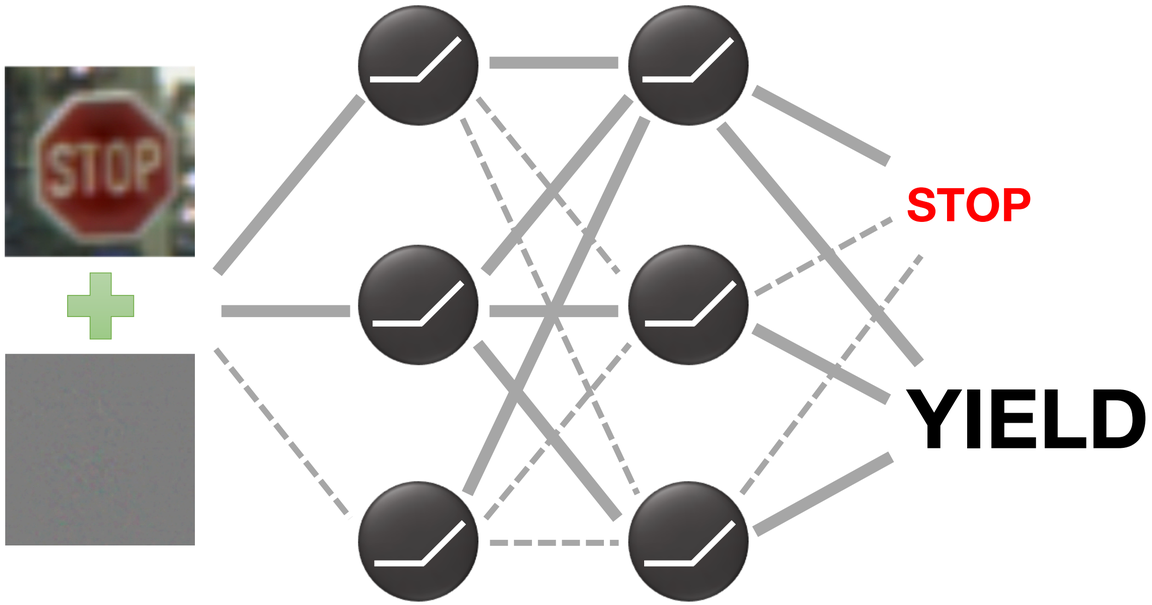
Goal: **Guarantee** that trained model has **desirable behavior**

→

Model ReLU with **Binary** variables + Linear **Inequalities**





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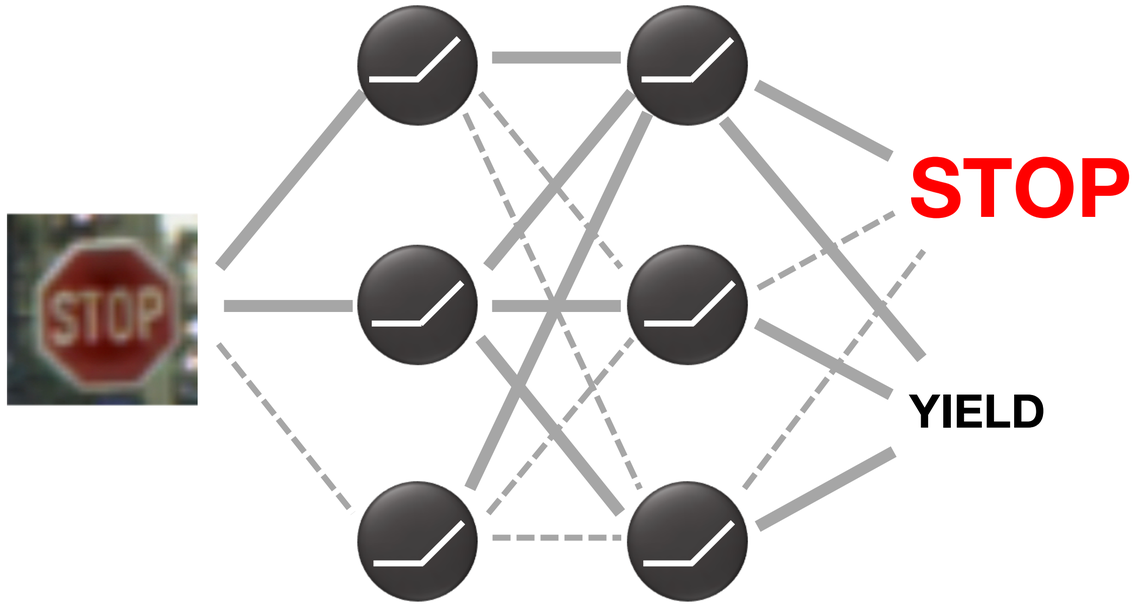

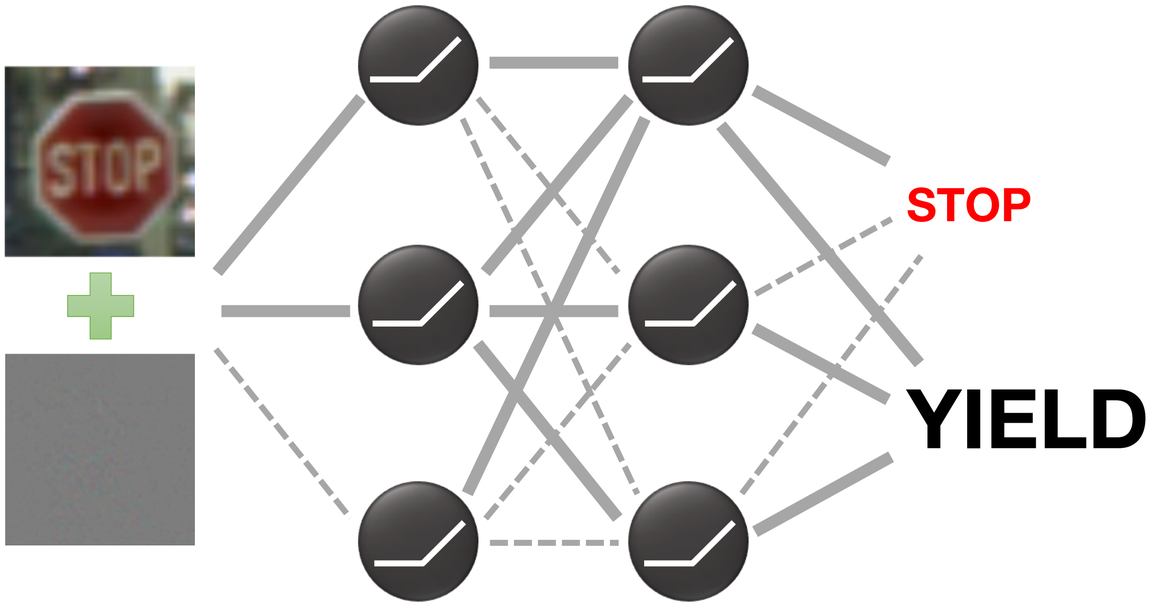

Safety-Critical Machine Learning

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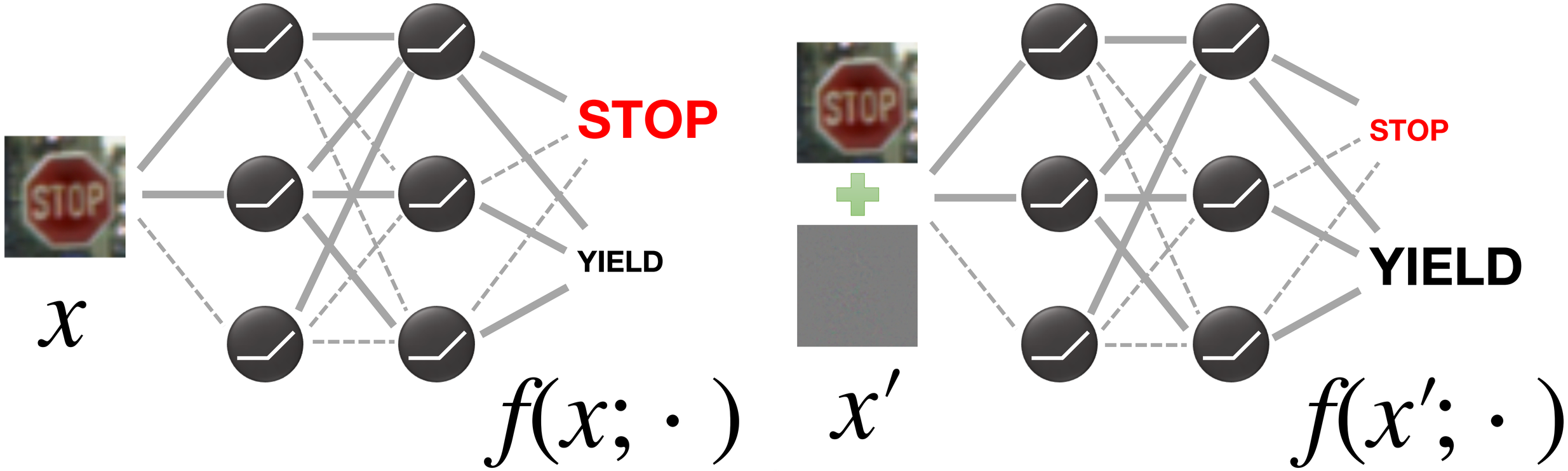
Verification Problem

prove $\nexists x'$ **close to** x

such that $f(x';$ **STOP**$) < f(x';$ **YIELD**$)$



Forest Harvesting

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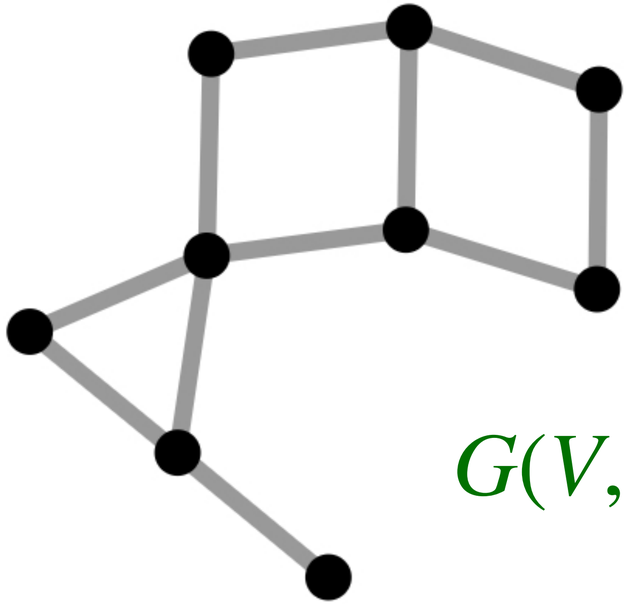
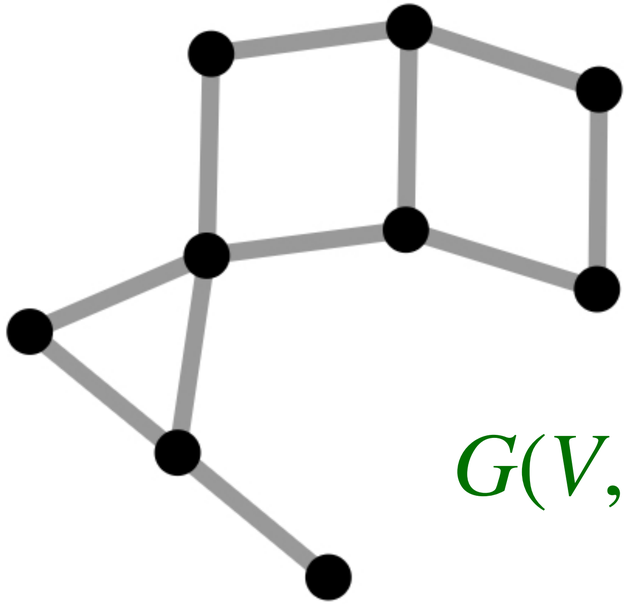


$G(V, E)$

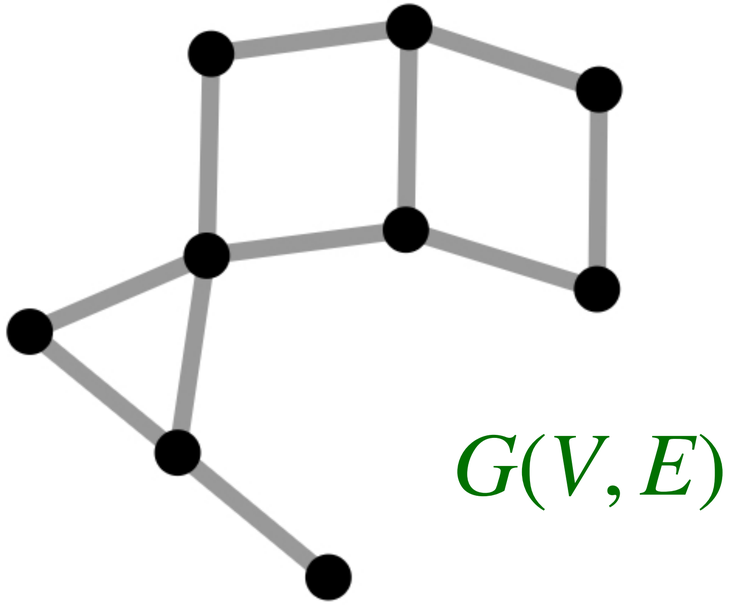
Forest Harvesting



$G(V, E)$

Forest Harvesting

Goal: Harvest subset of parcels to maximize **revenue**; pay **cost** for harvesting adjacent parcels



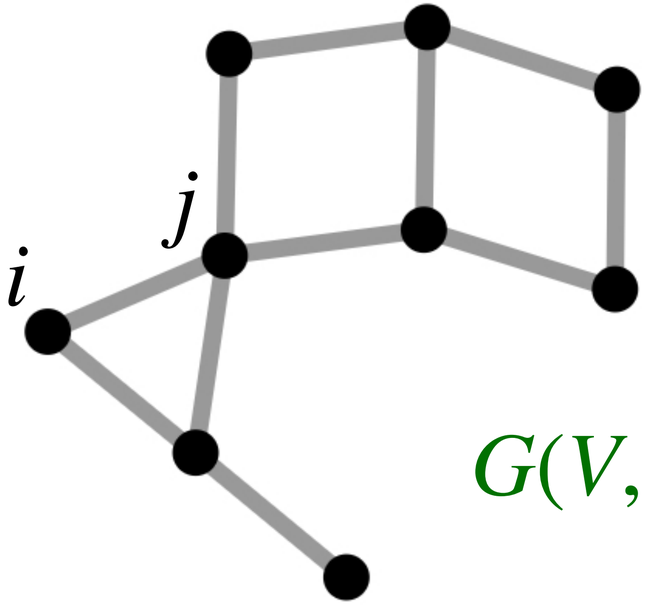
Forest Harvesting

Goal: Harvest subset of parcels to maximize **revenue**; pay **cost** for harvesting adjacent parcels

$$\textbf{maximize} \sum_{i \in V} r_i x_i - \sum_{(i,j) \in E} c_{ij} y_{ij}$$

$$\textbf{subject to } x_i + x_j - y_{ij} \leq 1$$

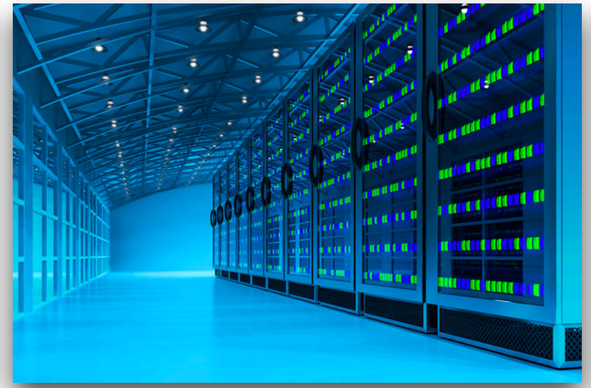
$$x \in \{0,1\}^n, y \in \{0,1\}^m$$



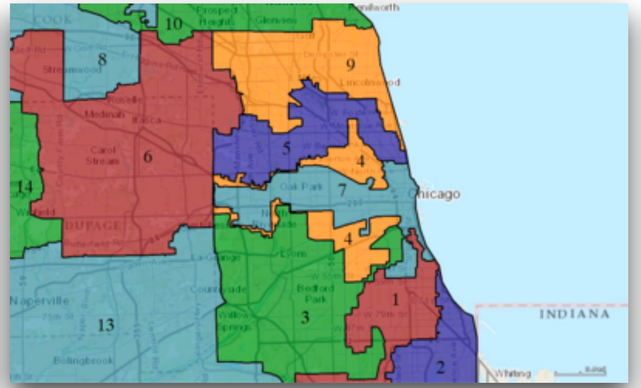
$G(V, E)$

Auction Design

Data Center Management



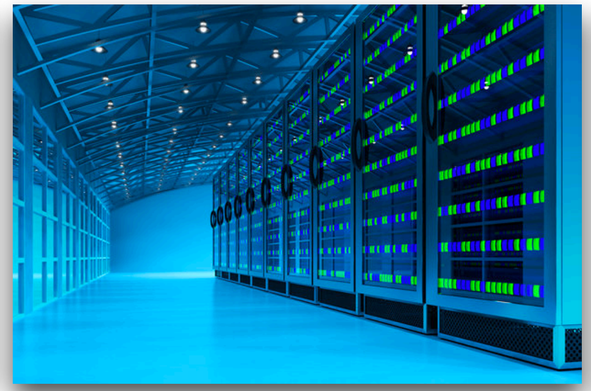
Political Districting



Kidney Exchange

Auction Design

Data Center Management



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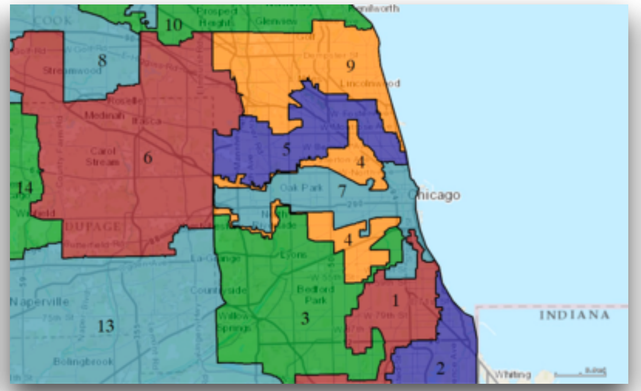

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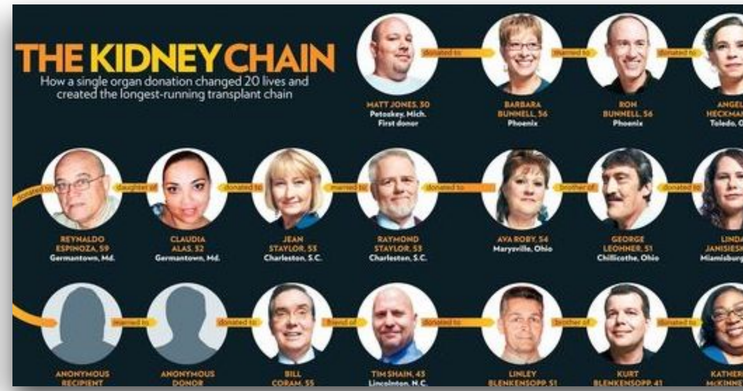
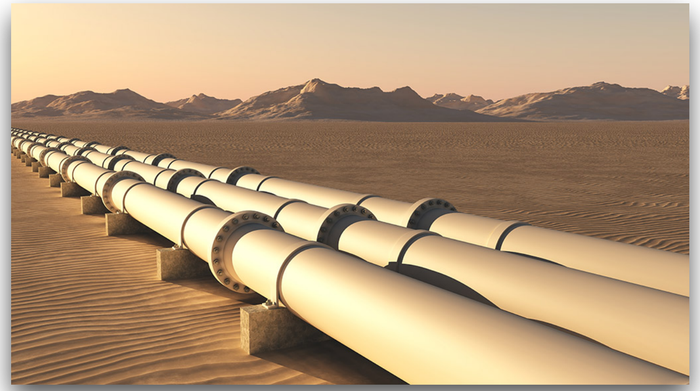
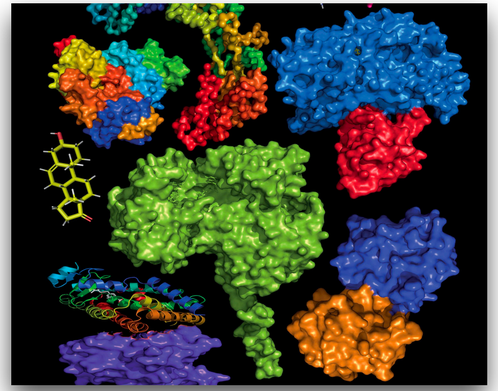


Energy Systems



Scientific Discovery

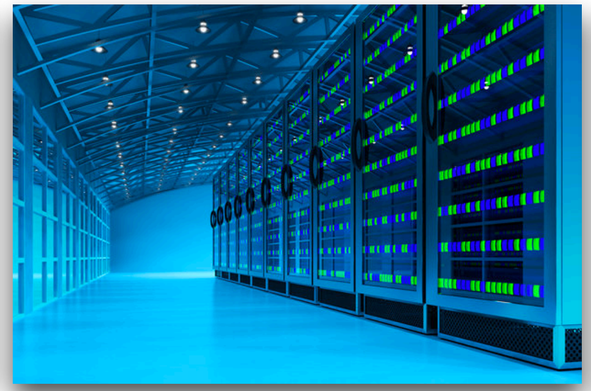


Ridesharing

Cancer Therapeutics

Auction Design

Data Center Management



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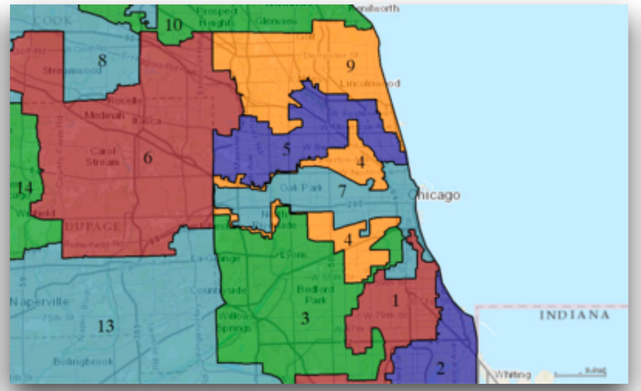

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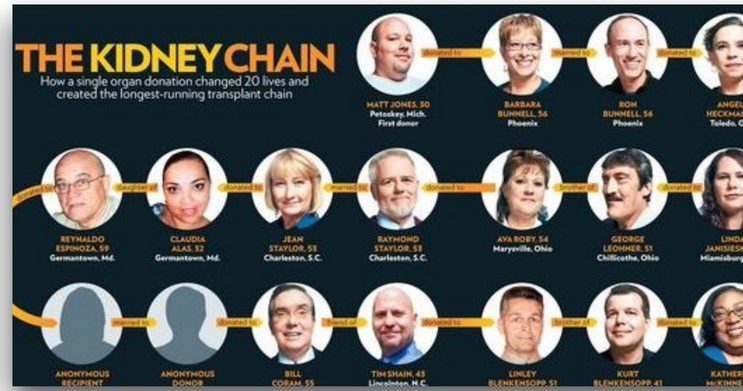

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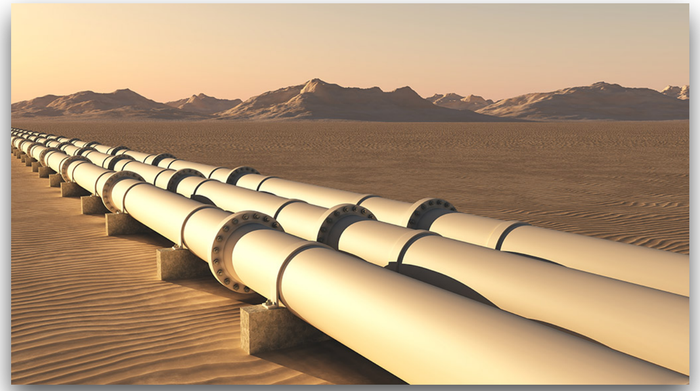

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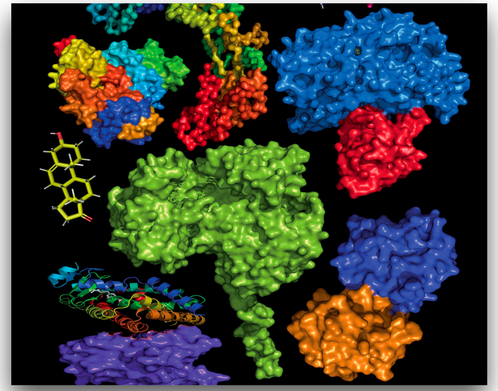


Ridesharing

Cancer Therapeutics

Airline Scheduling

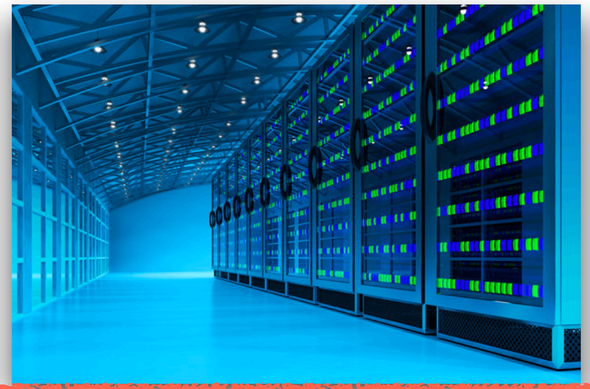
Conservation Planning

Disaster Response

College Admissions

Auction Design

Data Center Management



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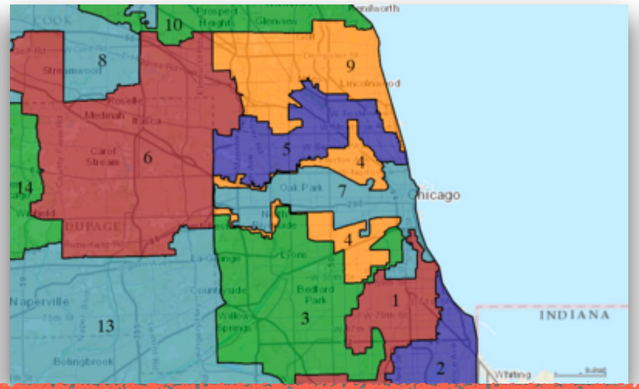

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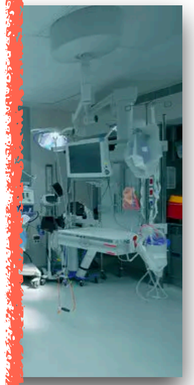

> 50% of INFORMS Edelman Award winners use Discrete Optimization

→ **Billions** ($) in savings/profit

George Nemhauser, Plenary at EURO INFORMS, 2013

Data Center Resource Management

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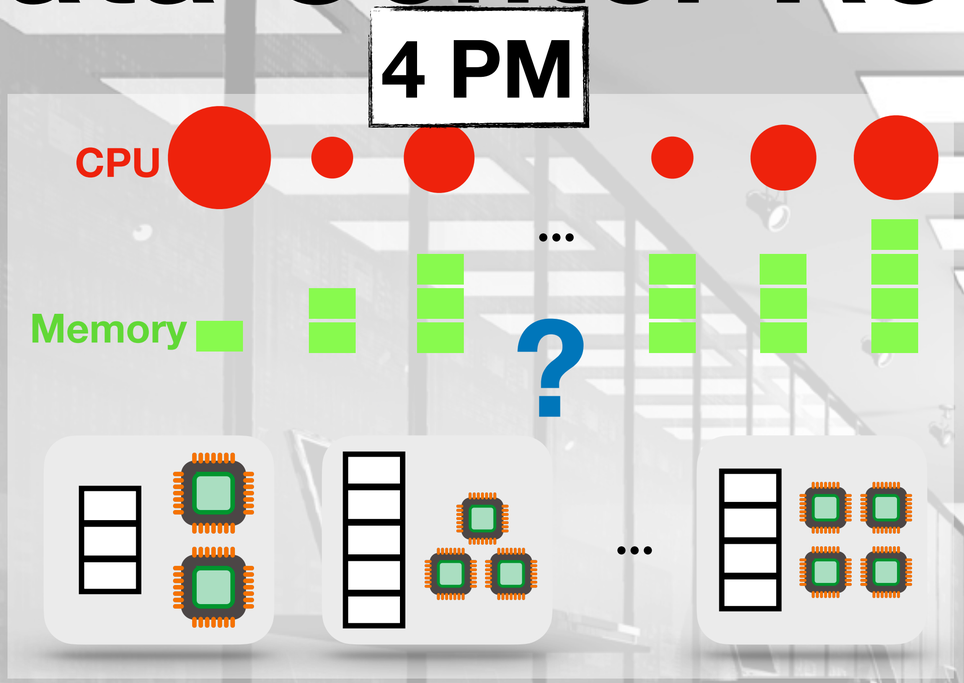

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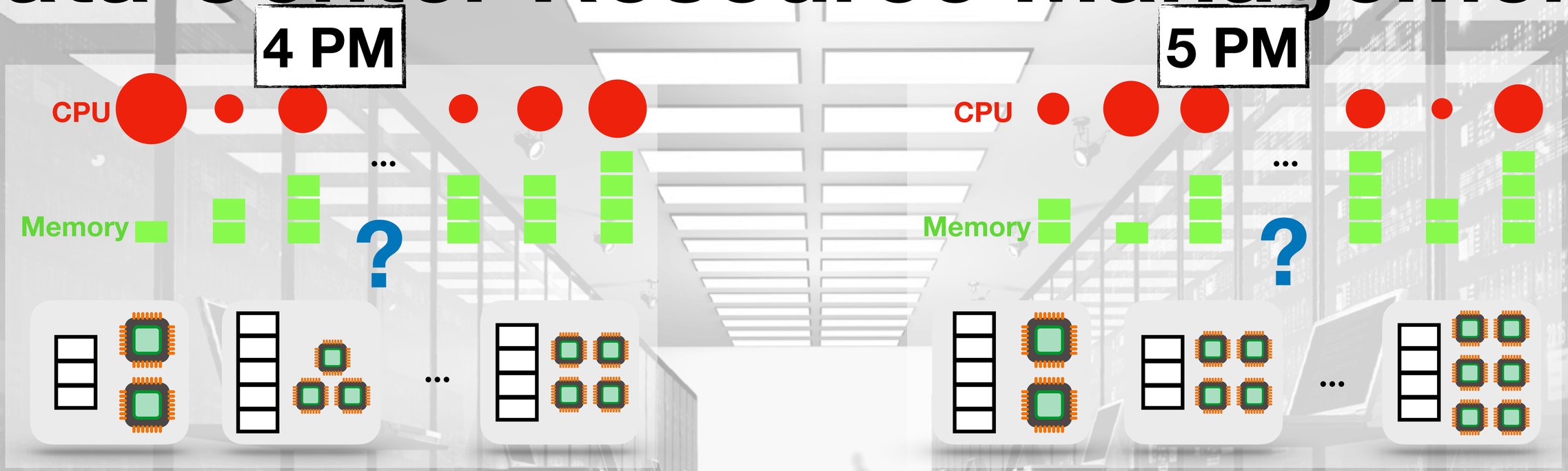

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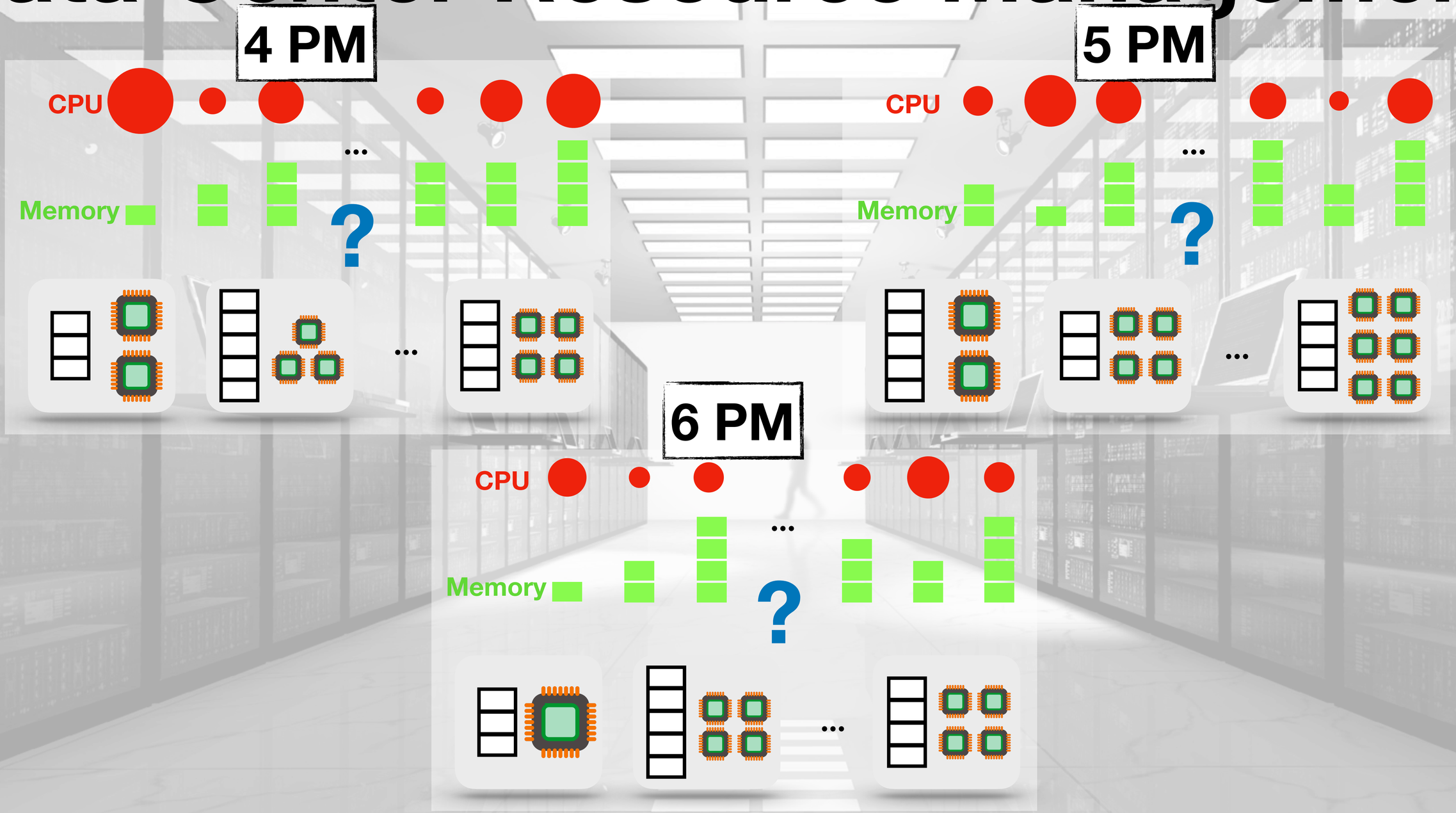

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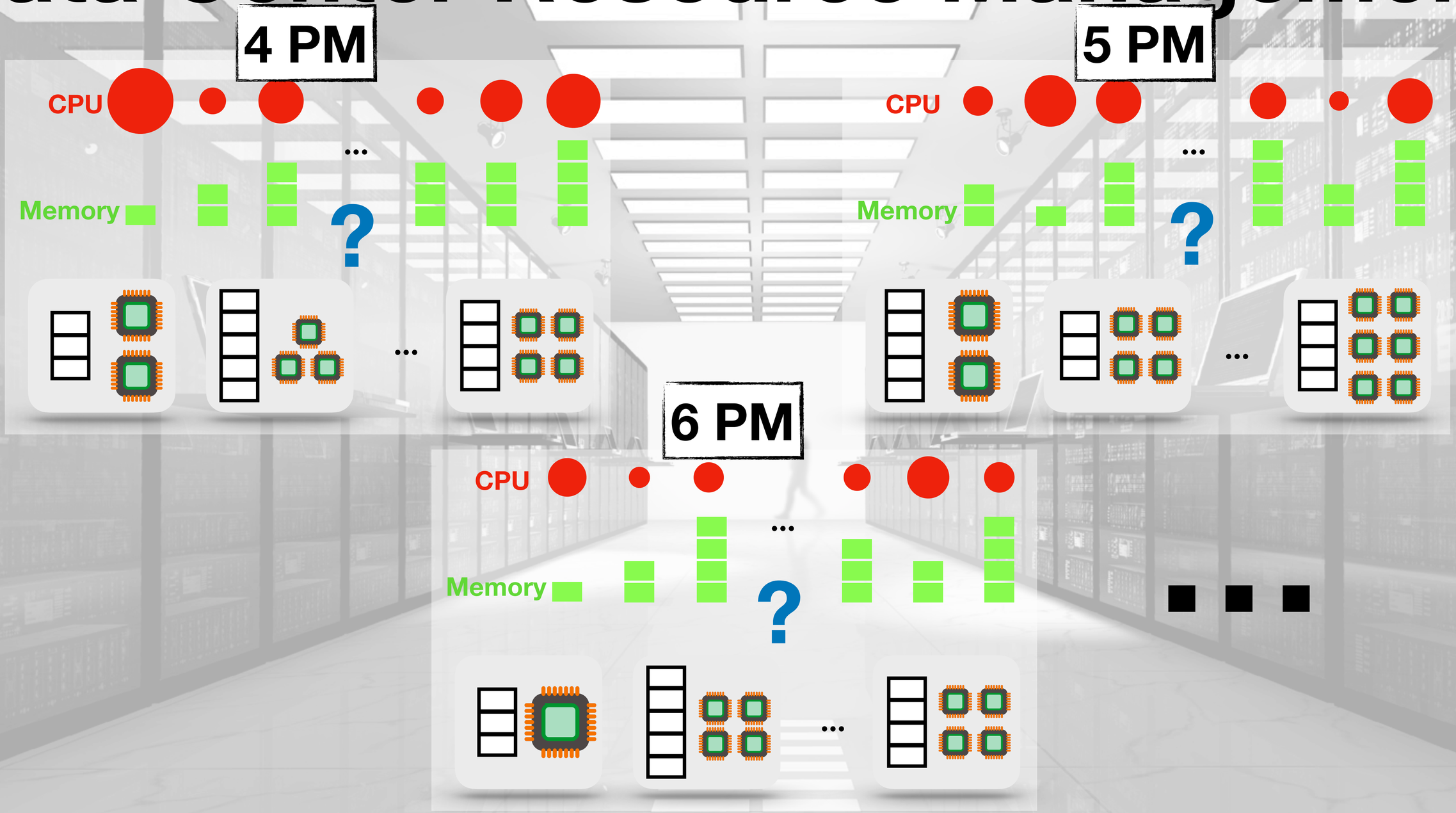

Tackling NP-Hard Problems

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Exhaustive Search	**Tight formulations** Powerful **Branch-and-Bound** solvers

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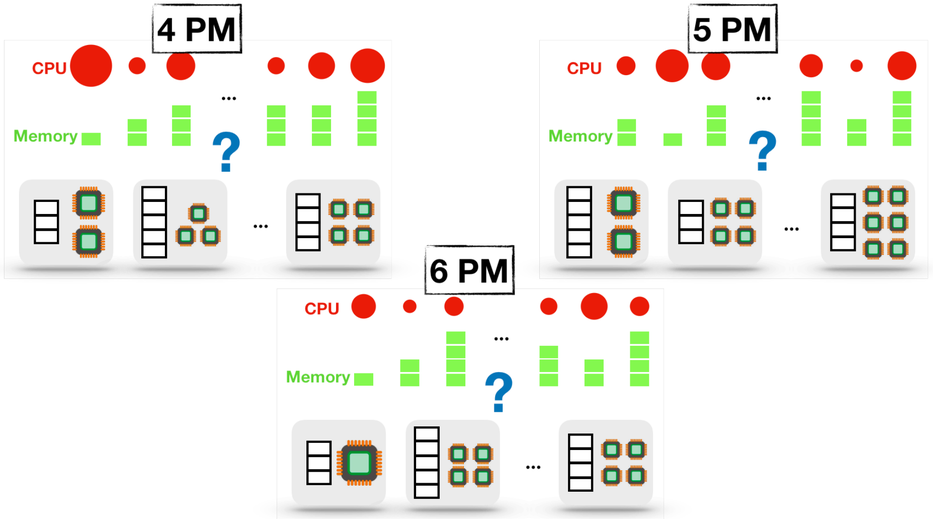

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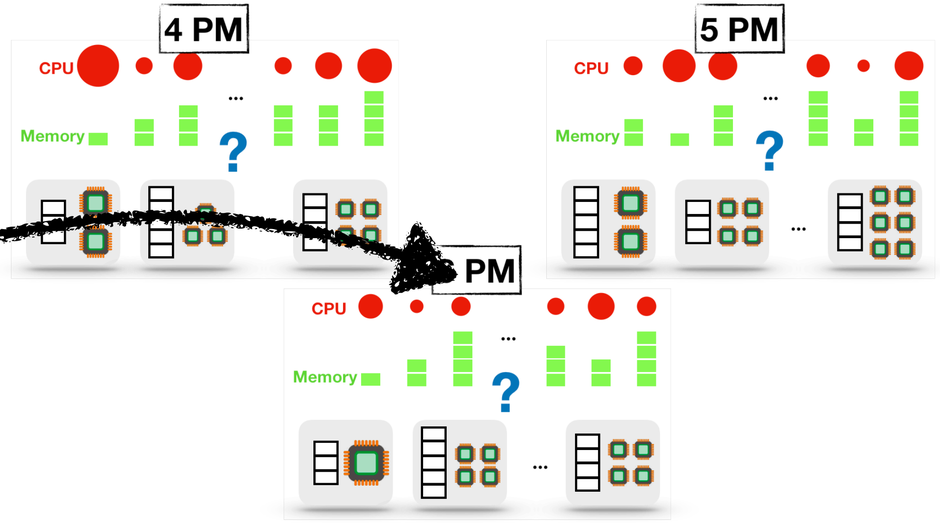

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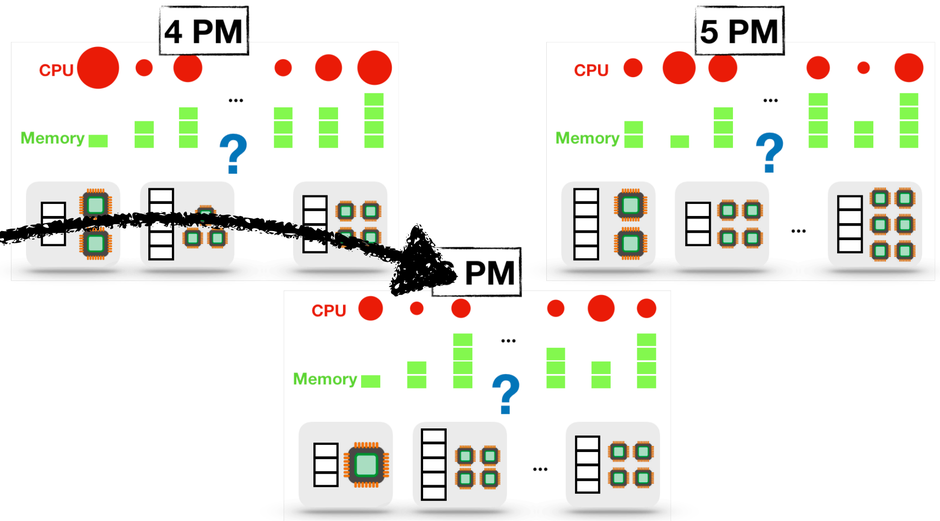

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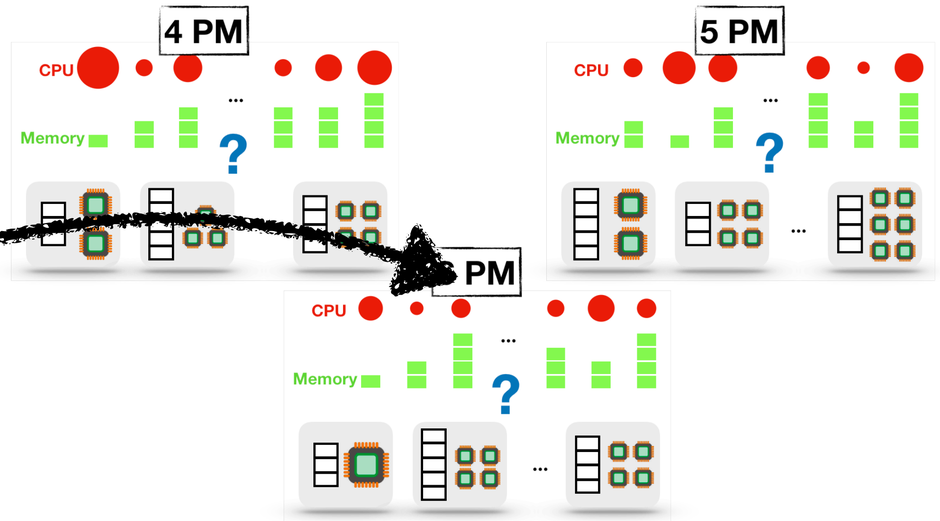

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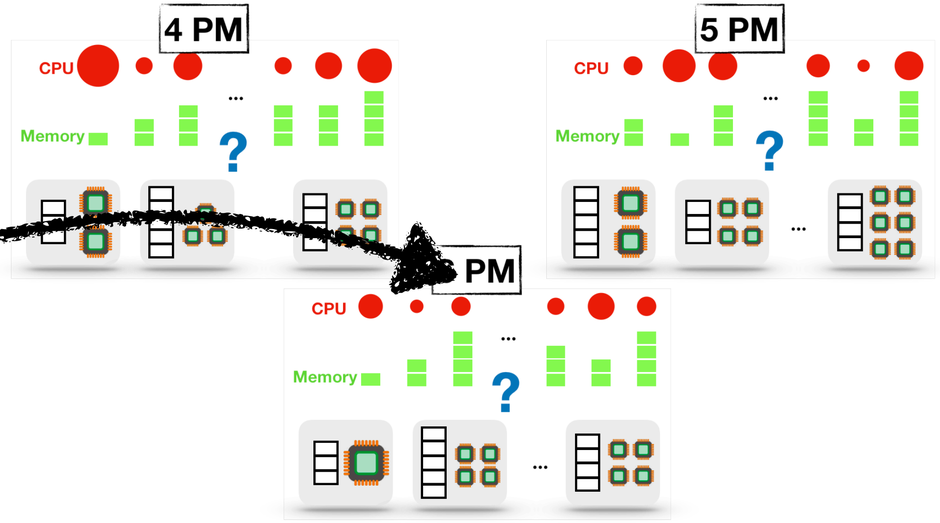

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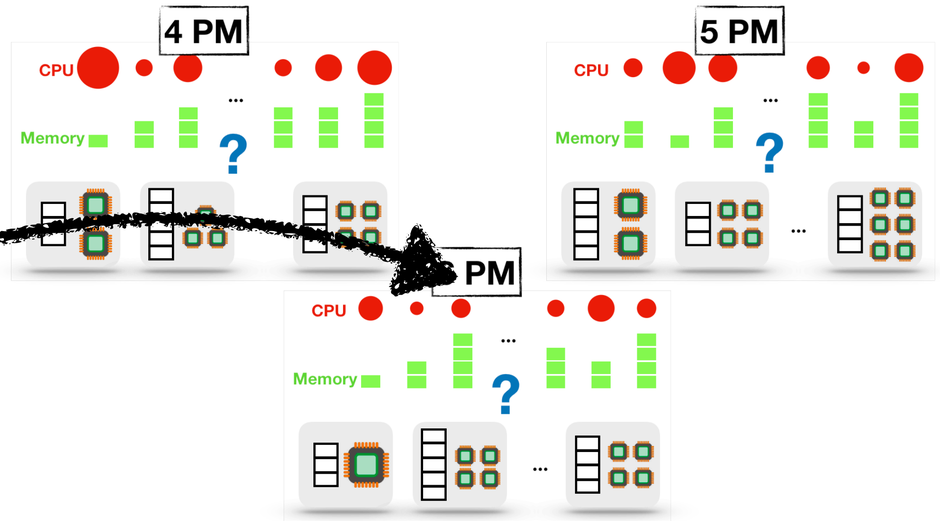

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Paradigm	Customization via…
	Problem-Specific Bounding functions or **search rules**
	Make explicit **assumptions** on input distribution and **redesign algo.**
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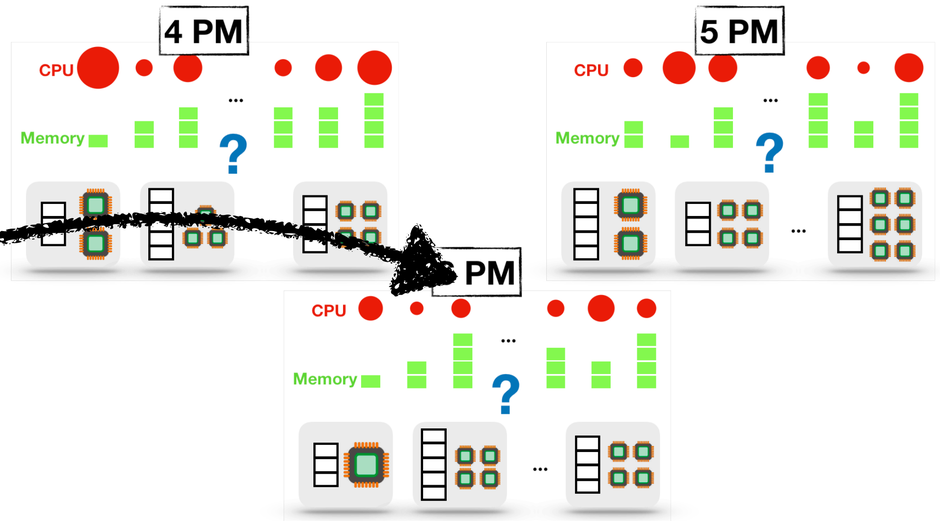
ANSWER:
Manual intellectual/ experimental **effort** required

How do you **tailor** the algorithm to **YOUR** instances?

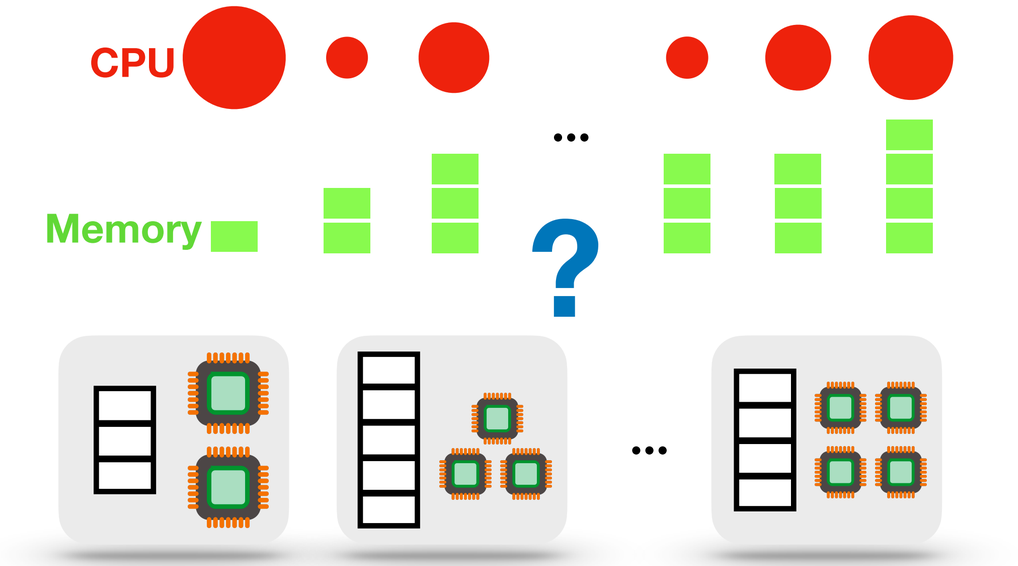


Opportunity

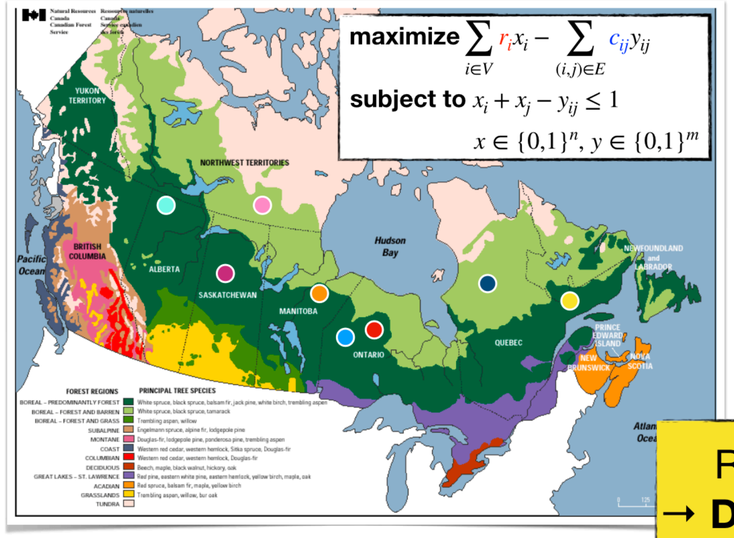
Parts 2-5 of this tutorial

Automatically tailor algorithms to a **family** of **instances**

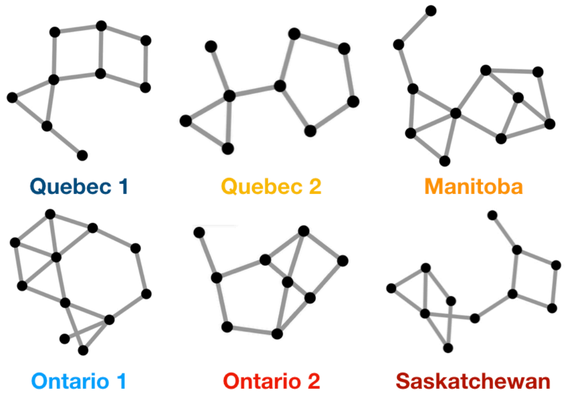
Data Center Resource Management



Forest Harvesting



and many more…



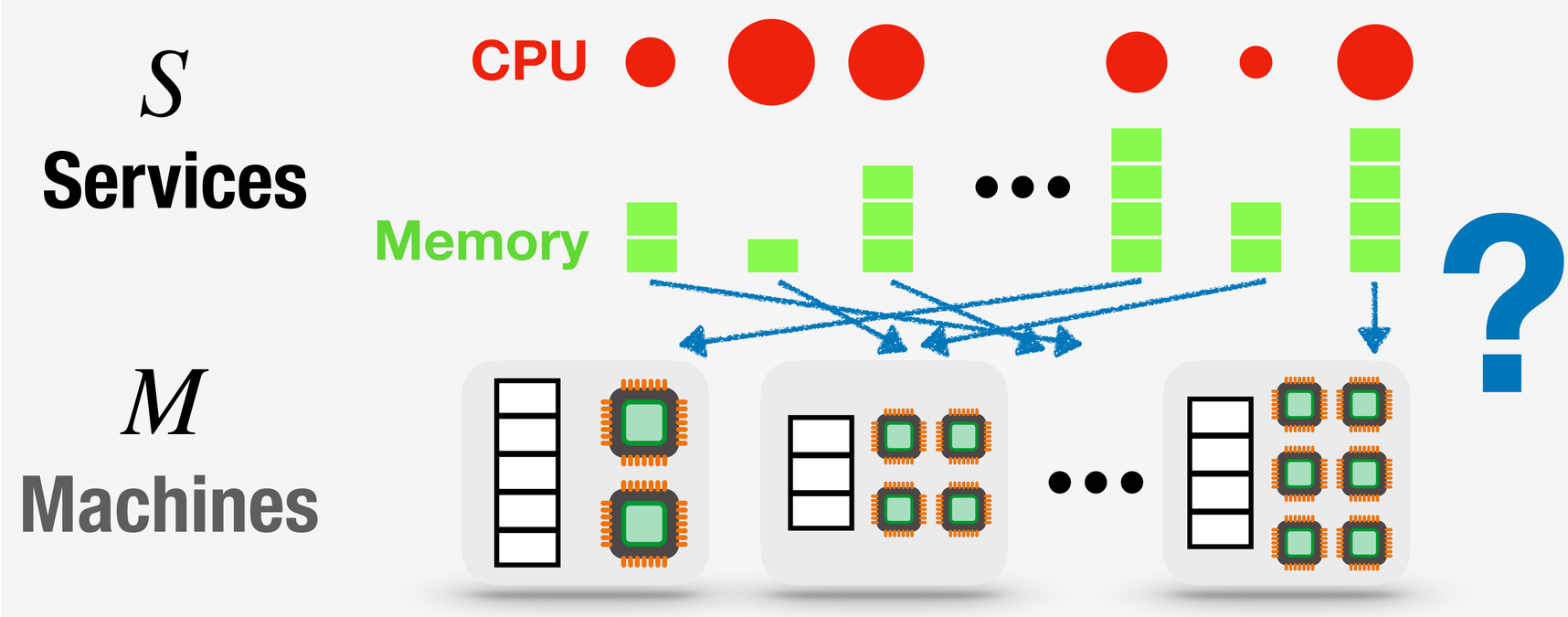
Revenue varies **over time**
→ **Different** instances, **same** problem

$y_m = 1$ if machine m is used

$x_{s,m} = 1$ if service s runs on m

$x \in \{0,1\}^{S \times M}, y \in \{0,1\}^M$

$$\textbf{minimize} \sum_{m=1}^{M} y_m$$



Constraints:

Each service on one machine only

$$\sum_{m=1}^{M} x_{s,m} = 1 \quad \forall s$$

$$y_m \geq x_{s,m} \quad \forall s, m$$

Machine is "ON" if a job is assigned to it

Memory capacity

$$\sum_{s=1}^{S} \textbf{mem}(s) \cdot x_{s,m} \leq \textbf{cap-mem}(m) \quad \forall m$$

$$\sum_{s=1}^{S} \textbf{cpu}(s) \cdot x_{s,m} \leq \textbf{cap-cpu}(m) \quad \forall m$$

Processor capacity

$y_m = 1$ if machine m is used

$x_{s,m} = 1$ if service s runs on m

$x \in \{0,1\}^{S \times M}, y \in \{0,1\}$

minimize $\sum_{m=1}^{M} y_m$

Where does this information come from?

Constraints:

Each service on one machine only

$$\sum_{m=1}^{M} x_{s,m} = 1 \quad \forall s$$

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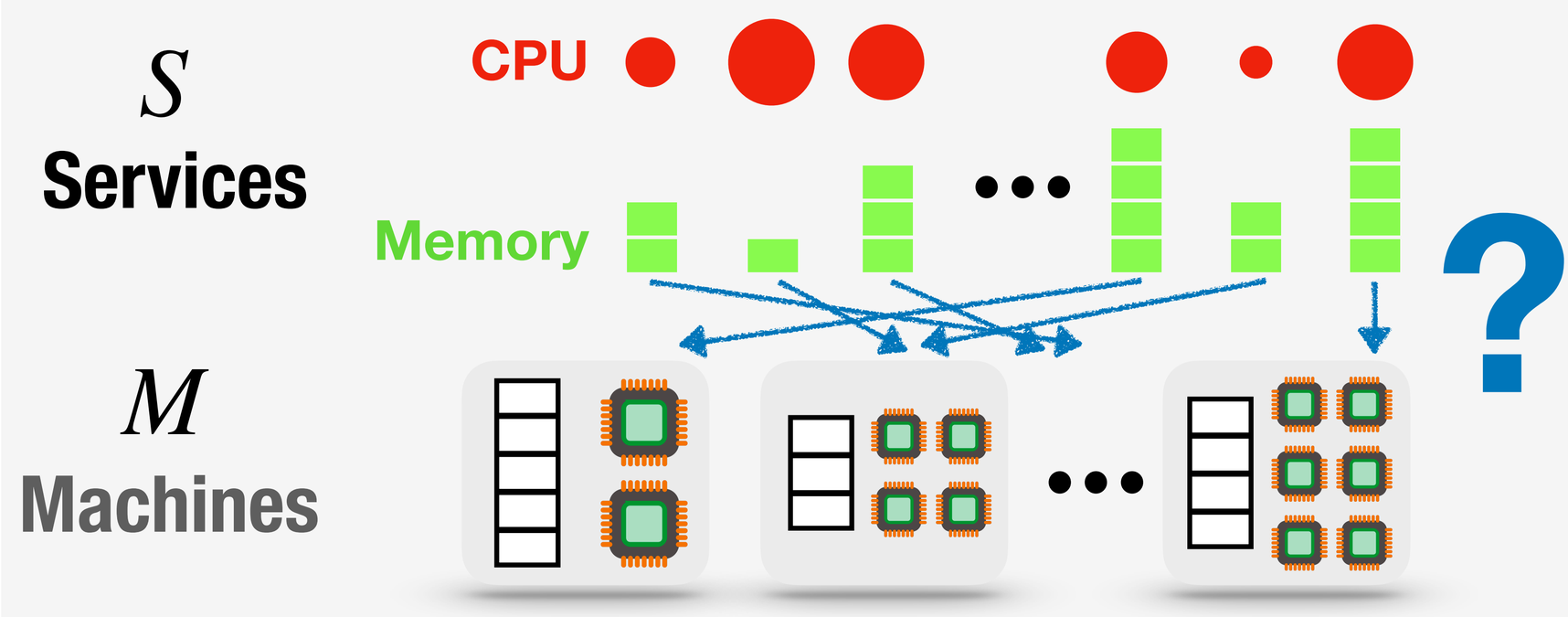

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Processor capacity

ML model for CPU usage:

$\textbf{cpu}(s) = \textbf{model}_\theta(\textbf{features}(s))$

Opportunity

Part 6 of this tutorial

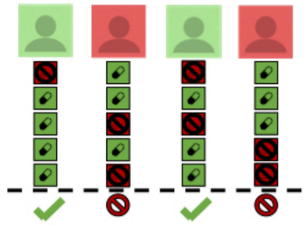
Decision-Focused Learning:

ML models that accurately predict parameters of optimization problems

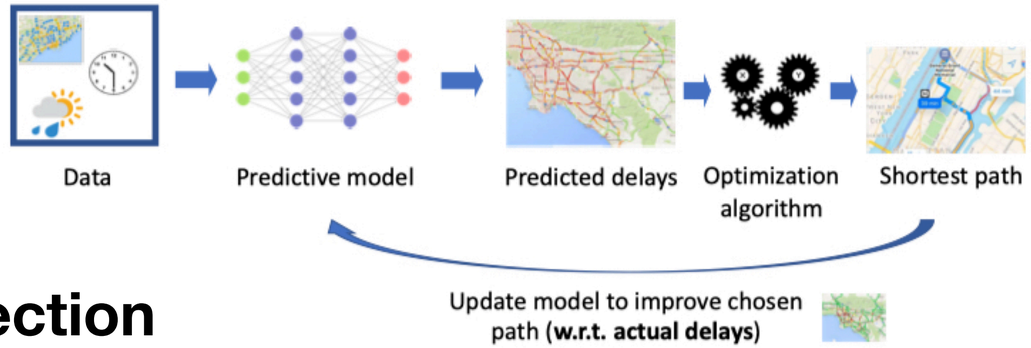
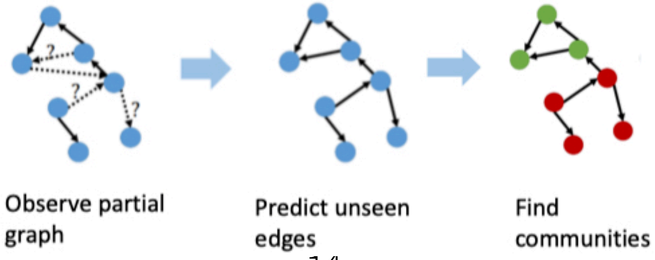
Tuberculosis Treatment

- **Predict** if patients will miss daily dose
- **Optimize** health worker visits subject to knapsack constraints (LP)

- More in our paper [Killian et al, KDD 2019]



Shortest paths with predictions



Community Detection